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FISCAL YEAR 1996 SUMMARY REPORT OF THE NOAA ATMOSPHERIC SCIENCES MODELING DIVISION SUPPORT TO THE U.S. ENVIRONMENTAL PROTECTION AGENCY

Evelyn M. Poole-Kober
Herbert J. Viebrock
(Editors)

Atmospheric Sciences Modeling Division
Research Triangle Park, North Carolina

Air Resources Laboratory
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NOTICE

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PREFACE

This document summarizes the Fiscal Year 1996 research and operational activities of the Atmospheric Sciences Modeling Division (ASMD), Air Resources Laboratory, working under Interagency Agreements EPA DW13937039 and DW13937252 between the U.S. Environmental Protection Agency (EPA) and the National Oceanic and Atmospheric Administration (NOAA). The summary includes descriptions of research and operational efforts in air pollution meteorology, air pollution control activities, and abatement and compliance programs.

Established in 1955, the Division serves as the vehicle for implementing the agreements with the EPA, which funds the research efforts in air pollution meteorology. ASMD conducts research activities in-house and through contract and cooperative agreements for the National Exposure Research Laboratory and other EPA groups. With a staff consisting of NOAA, EPA, and Public Health Service Commissioned Corps personnel, ASMD also provides technical information, observational and forecasting support, and consulting on all meteorological aspects of the air pollution control program to many EPA offices, including the Office of Air Quality Planning and Standards. The primary groups within ASMD are the Atmospheric Model Development Branch, Fluid Modeling Branch, Modeling Systems Analysis Branch, Applied Modeling Research Branch, and Air Policy Support Branch. The staff is listed in Appendix F. Acronyms, publications, and other professional activities are listed in the remaining appendices.

Any inquiry on the research or support activities outlined in this report should be sent to the Director, Atmospheric Sciences Modeling Division (MD-80), Environmental Protection Agency, Research Triangle Park, NC 27711.

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ABSTRACT. During Fiscal Year 1996, the Atmospheric Sciences Modeling Division provided meteorological and modeling support to the U.S. Environmental Protection Agency. This ranged from the conduct of research studies and model applications to the provision of advice and guidance. Research efforts emphasized the development and evaluation of air quality models using numerical and physical techniques supported by field studies. Among the significant research studies were the continued development and evaluation of Models-3; development of a regional particulate model; development and application of air quality models for mercury, dioxin, and heavy metals; conduct of dry deposition field studies; conduct of convection tank experiments of the plume penetration of elevated inversions; and evaluation of models for the dispersion of pesticides.

1. INTRODUCTION

In Fiscal Year 1996, the Atmospheric Sciences Modeling Division (ASMD) continued its commitment for providing goal-oriented, high-quality research and development, and operational support to the U.S. Environmental Protection Agency (EPA). Using an interdisciplinary approach emphasizing integration and close cooperation with the EPA and public and private research communities, the Division's primary efforts were studying processes affecting dispersion of atmospheric pollutants, modeling pollutant dispersion on all temporal and spatial scales, and developing multi-media model frameworks in a high computing and communications environment. The technology and research products developed by the Division are transferred to the national and international user communities in the public and private sectors. Section 2.1 discusses Division participation in international activities, while Sections 2.2 through 2.5 outline the Division research activities in support of the short- and long-term needs of the EPA and the environmental community. Section 2.6 discusses Division support to the operational programs and general air quality model user community.

2. PROGRAM REVIEW

2.1 Office of the Director

The Office of the Director provides direction, supervision, program management, and administrative support in performing the Atmospheric Sciences Modeling Division's mission and in achieving its goals of advancing the state of the atmospheric sciences and enhancing the protection of the environment. The Director's Office also engages in several domestic and international research exchange activities.

2.1.1 NATO Committee on Challenges of Modern Society

The North Atlantic Treaty Organization (NATO) Committee on Challenges of Modern Society (CCMS) was established in 1969 with the mandate to examine how to improve, in every practical way, the exchange of views and experience among the Allied countries in the task of creating a better environment for their societies. The Committee considers specific problems of the human environment with the deliberate objective of stimulating action by member governments.

The Committee's work is carried out on a decentralized basis through pilot studies, discussions on environmental issues, and fellowships.

2.1.1.1 International Technical Meetings

The Division Director serves as the United States representative on the Scientific Committee for International Technical Meetings (ITMs) on Air Pollution Modeling and Its Application, sponsored by NATO/CCMS. A primary activity within the NATO/CCMS Pilot Study on Air Pollution Control Strategies and Impact Modeling is organizing a symposium every two years that deals with various aspects of air pollution dispersion modeling. The meetings are rotated among different NATO members, with every third ITM held in North America and the two intervening ITMs held in European countries.

The Division Director served as sponsor and conference chairman of the 21st NATO/CCMS International Technical Meeting held in Baltimore, Maryland, during November 6-10, 1995; the proceedings were published by Plenum Press (Gryning and Schiermeier, 1996). The NATO/CCMS Scientific Committee selected Clermont- Ferrand, France, as the site for the 22nd International Technical Meeting to be held during June 2-6, 1997.

2.1.1.2 Coastal Urban Air Pollution Study

The Division Director serves as the United States representative on the International Oversight Committee for the NATO/CCMS Pilot Study on Urban Pollutant Dispersion near Coastal Areas. This pilot study, sponsored by Greece, originated in a workshop held in Athens during February 1992. The purpose is to understand the causes of high air pollution episodes in coastal urban areas and to devise strategies to mitigate pollution problems caused by vehicular and industrial emissions in these areas. A NATO/CCMS advanced research workshop was held during May 1993 to design a reference experiment in a coastal urban area to collect relevant ambient measurements and emissions for use in evaluation of existing urban dispersion models and for understanding the atmospheric boundary layer at the interface of land and water. A workshop summary was published (Melas *et al*., 1995). The final report of the pilot study will be presented at a NATO/CCMS Plenary Meeting in Brussels, Belgium, in April 1997.

2.1.2 United States/Japan Environmental Agreement

The Division Director serves as the United States Co-Chairman of the Air Pollution Meteorology Panel under the United States/Japan Agreement on Cooperation in the Field of Environment. The purpose of this 1975 agreement is to facilitate, through mutual visits and reciprocal assignments of personnel, the exchange of scientific and regulatory research results pertaining to control of air pollution. Although no reciprocal visits were made in FY-1996, interactions were maintained through correspondence and exchanges of research findings.

2.1.3 United States/Russia Joint Environmental Committee

The Division Director serves as the United States Co-Chairman of the United States/Russia Working Group 02.01-10 on Air Pollution Modeling, Instrumentation, and Measurement Methodology, and as Co-Leader of the United States/Russia Project 02.01-11 on Air Pollution Modeling and Standard Setting. The purpose of the 1972 Nixon-Podgorny Agreement forming the US/USSR Joint Committee on Cooperation in the Field of Environmental Protection is to promote, through mutual visits and reciprocal assignments of personnel, the sharing of scientific and regulatory research results related to the control of air pollution. Activities under this agreement have been extended to also comply with the 1993 Gore-Chernomyrdin Agreement forming the United States/ Russia Commission on Economic and Technological Cooperation. There are four Projects under Working Group 02.01-10:

Project 02.01-11: Air Pollution Modeling and Standard Setting
Project 02.01-12: Instrumentation and Measurement Methodology
Project 02.01-13: Remote Sensing of Atmospheric Parameters
Project 02.01-14: Statistical Analysis Methodology and Air Quality Trend Assessment.

Progress under this Working Group continued during FY-1996. The annual Working Group meeting at the Main Geophysical Observatory in St. Petersburg, Russia, was delayed until July 1997. Two National Research Council (NRC) research associateships were completed during the year. These included a Russian expert in remote sensing assigned to the EPA Characterization Research Division in Las Vegas, Nevada, and a Russian scientist at the Division's Fluid Modeling Facility in Research Triangle Park, North Carolina.

2.1.4 Meteorological Coordinating Committees

2.1.4.1 Federal Meteorological Committee

The Division Director serves as the Agency representative on the Federal Committee for Meteorological Services and Supporting Research (FCMSSR). The Committee is composed of representatives from 14 Federal government agencies and is chaired by the Under Secretary of Commerce for Oceans and Atmosphere, who is also the NOAA Administrator. FCMSSR was established in 1964 with high-level agency representation to provide policy guidance to the Federal Coordinator for Meteorology, and to resolve agency differences that arise during coordination of meteorological activities and the preparation of Federal plans in general.

2.1.4.2 Interdepartmental Meteorological Committee

The Division Director serves as the Agency representative on the Interdepartmental Committee for Meteorological Services and Supporting Research (ICMSSR). The Committee, composed of representatives from 14 Federal government agencies, was formed in 1964 under Public Law 87-843 and OMB Circular A-62 to provide the Executive Branch and the Congress with a coordinated, multi-agency plan for government meteorological services and for those research and development programs that directly support and improve these services. The Committee prepared the annual Federal Plan for Meteorological Services and Supporting Research (U.S. Department of Commerce, 1996). A Division scientist serves on the ICMSSR Working Group for Atmospheric Transport and Diffusion and four other Division scientists served on an ICMSSR panel to develop a National Agenda for Meteorological Services and Supporting Research (U.S. Department of Commerce, in press).

2.1.5 United States Weather Research Program

The Division Director serves as the Agency representative on the interagency working group for the United States Weather Research Program (USWRP). This initiative is designed to (1) increase benefits to the Nation from the substantial investment in modernizing the public weather warning and forecast system in the United States; (2) improve local and regional forecasts and warnings; (3) address critical weather-related scientific issues; and (4) coordinate government, university, and private sector efforts. The program is broad in scope, encompassing the full range of atmospheric processes that are part of weather, including dynamics, thermodynamics, synoptics, cloud physics, atmospheric chemistry, electricity, and radiation, as well as their effects on hydrology.

2.1.6 NAS/NRC Board on Atmospheric Sciences and Climate

The Division Director serves as the Agency liaison to the Board on Atmospheric Sciences and Climate (BASC) of the National Research Council, National Academy of Sciences. The BASC activity that most closely relates to the work of the Division is the Panel on Atmospheric Aerosols. Specifically, the panel will review existing and new evidence regarding anthropogenic and natural aerosol-producing processes; their sources, characteristics and distribution; their transport and removal; and their quantified effects on atmospheric processes and on the global and regional radiation forcing of the climate system. The panel will advise regarding the observation, monitoring, and research strategies needed to understand atmospheric processes and aerosol characteristics important in weather and air pollution research.

2.1.7 OSTP/NSTC Committee on Computing, Information, and Communications

The Division Director serves as the alternate Agency member to the Committee on Computing, Information, and Communications (CCIC) of the National Science and Technology Council, Office of Science and Technology Policy. The mission of the Committee is to "accelerate the evolution of existing technology and nurture innovation that will enable universal, accessible, and affordable application of information technology to enable America's economic and national security in the 21st century" (U.S. Office of Science and Technology Policy, 1995). This mission is achieved through six strategic focus areas: global-scale information infrastructure technologies; high performance/scalable systems; high confidence systems; virtual environments; user-centered interfaces and tools; and human resources and education. The Committee serves as the National Coordination Office for the High Performance Computing and Communications (HPCC) program in which this Division has a major role.

2.1.8 Standing Air Simulation Work Group

The Division Director serves as the Agency Office of Research and Development (ORD) representative to the Standing Air Simulation Work Group (SASWG), which serves as a forum for issues relating to air quality simulation modeling of criteria and other air pollutants from point, area, and mobile sources. Its scope encompasses policies, procedures, programs, model development, and model application. The work group fosters consensus between the Agency and the State and local air pollution control programs through semi-annual meetings of members representing all levels of enforcement.

2.1.9 AMS Glossary of Meteorology

The Division is participating in multi-agency funding of the updating and revision of the Glossary of Meteorology by the American Meteorological Society (AMS). Under sponsorship of the National Science Foundation (NSF), the AMS will review the existing entries in the 1959 edition of the Glossary and revise and update the listings resulting in a potential doubling of the number of entries. The new Glossary will be published in both print and CD-ROM formats.

2.1.10 European Monitoring and Evaluation Program

A Division scientist serves as the United States representative to the European Monitoring and Evaluation Program (EMEP) that oversees the cooperative program for monitoring and evaluation of the long-range transmission of air pollutants in Europe. The primary goal of EMEP is to use regional air quality models to produce assessments evaluating the influence of one country's emissions on another country's air concentrations or deposition. The emphasis is shifting from acidic deposition to ozone. The United States and Canadian representatives report on North American activities related to long-range transport. The Division scientist also evaluates European studies of special relevance to the program, providing technical critiques of the EMEP work during formal and informal interactions; and develops and coordinates such programs with EMEP as the modeling studies of the Modeling Synthesizing Center West (MSC-W) at the Norwegian Meteorological Institute in Oslo, Norway.

2.1.11 Clean Air Act Amendments of 1990 Section 812 Assessment Work Group

A Division scientist is a member of the 812 Assessment Work Group, in coordination with the EPA Office of Program Assessment and Review and the EPA Office of Policy Planning and Evaluation, with responsibility for developing approaches to assess regional air quality and acidic deposition. The responsibilities of this working group are to produce a retrospective assessment of the benefits and costs of the Clean Air Act (CAA) of 1970 and a prospective assessment of the benefits and costs of the Clean Air Act Amendments (CAAA) of 1990, assuming full implementation. Work in FY-1996 emphasized peer review of the retrospective assessment and development, and review of emission projections for the prospective study.

2.1.12 Chesapeake Bay Program Air Subcommittee and Chesapeake Bay Program Modeling Subcommittee

A Division scientist is a member of the Air Subcommittee, a working subcommittee of the Chesapeake Bay Program. Previously this subcommittee was an advisory group to the Implementation Committee. The subcommittee has responsibility for advice and leadership on issues of atmospheric deposition to the watershed and the Bay, on overseeing application of the Regional Acid Deposition Model (RADM), and in dealing with the influence of atmospheric deposition on Bay restoration efforts. The Air Subcommittee also works with other Chesapeake Bay committees to define the top priority air quality scenarios to be simulated by RADM. The Division scientist is also an ex officio member of the Modeling Subcommittee of the Implementation Committee. This subcommittee has responsibility for overseeing the application of water quality models and coordinating the linkage of RADM with those models and the interpretation of the findings. Work in FY-1996 focused on creation of RADM predictions at 20-km resolution of the estimated effects of 1990 CAAA potential oxidant-related controls and feasible controls on the nitrogen deposition to the Chesapeake watershed basins and to the Bay.

2.1.13 Consortium for Advanced Modeling of Regional Air Quality

A Division scientist serves as an Agency representative to the Consortium for Advanced Modeling of Regional Air Quality (CAMRAQ). This consortium is composed of representatives from the Electric Power Research Institute, American Petroleum Institute, Pacific Gas and Electric, California Air Resources Board, Department of Energy, National Oceanic and Atmospheric Administration, Environmental Protection Agency, Department of Defense, Atmospheric Environment Service of Canada, Ontario Ministry of the Environment, and EUROTRAC (EUROpean experiment on the TRAnsport and transformation of trace atmospheric Constituents). The members of CAMRAQ share a mutual interest in making regional-scale atmospheric models usable tools for air quality and emergency response planning. They also share an interest in bringing the emerging power of high performance computing to regional air quality modeling. The goal of the consortium is to coordinate research and to form a basis for collaboration on projects that will enhance the ability of each to achieve their respective goals regarding atmospheric modeling. In FY-1996, a conceptual design was completed for a CAMRAQ Comprehensive Modeling System framework. This framework is also intended to be coordinated with the development of the EPA Third Generation Modeling System, Models-3.

2.1.14 National Acid Precipitation Assessment Program

A Division scientist serves as Chairman of the National Acid Precipitation Assessment Program (NAPAP) Subgroup on Processes and Deposition/Air Quality Modeling of the Atmospheric Effects Working Group, following the new mandate and organization of NAPAP under the 1990 CAAA. RADM application studies in support of EPA Congressionally-mandated reports helped to evaluate the effectiveness of the acidic deposition control program of the CAAA Title IV and helped determine the reductions in emissions that are associated with deposition rates needed to prevent adverse effects.

2.1.15 North American Research Strategy for Tropospheric Ozone

The North American Research Strategy for Tropospheric Ozone (NARSTO) is a research program with the goal of addressing outstanding issues regarding the understanding and management of tropospheric ozone and coordinating collaborative research among all North American organizations performing and sponsoring tropospheric ozone studies. Sponsors include the private sector and State, Provincial and Federal governments of the United States, Canada and Mexico. NARSTO was formally established in FY-1995. The Subcommittee on Air Quality Research of the Committee on Environment and Natural Resources (CENR) within the National Science and Technology Council (NSTC) will facilitate the coordination of NARSTO Federal research activities. Four technical teams have been established: Analysis and Assessment; Observations; Modeling and Chemistry; and Emissions. A first major goal of NARSTO is to produce in 1998 a scientific assessment of the state of tropospheric ozone science.

During FY-1996, the process for the 1998 NARSTO scientific assessment was established. A Division scientist was chosen to co-author one of the fifteen critical review papers that were commissioned to provide technical background to the NARSTO assessment group. The critical review will be on modeling and evaluation of advanced models.

2.1.16 Southern Oxidant Study

A Division scientist is a member of the Modeling and Model Science Team of the Southern Oxidant Study (SOS). Efforts are directed towards model evaluation using SOS data for the regional models coupled with urban models. As part of this work, the Division scientist was also a member of the 1995 Nashville/Middle Tennessee Ozone Study Planning Team. An experimental design was produced in FY-1995 (Tennessee Valley Authority, 1995). A Division scientist was a mentor for one of the aircraft experiments in the design plan. The scientist participated in the on-site aircraft experiment planning during the 1995 summer field campaign, and in data workshops providing first looks at the data in FY-1996.

2.1.17 International Task Force on Forecasting Environmental Change

A Division scientist is a member of the International Task Force on Forecasting Environmental Change that addresses the methodological and philosophical problems of forecasting under the expectation of significant structural changes in the behavior of physical, chemical or biological systems. In July 1996, the third of three planned workshops was held at the International Institute for Applied Systems Analysis in Laxenburg, Austria. At the workshop, potential chapters for a monograph were presented and reviewed and the outline of the monograph refined. Work is progressing on individual chapters for the monograph.

2.1.18 RADM Application Studies

Efforts during FY-1996 concentrated on completing several RADM application studies related to the 1997 Chesapeake Bay Agreement Reevaluation and analyzing RADM results in support of Regulatory Impact Statements mandated in the 1990 CAAA for ozone and visibility. Other applications are in progress, principally for the Chesapeake Bay and other coastal estuaries. The EPA Region 3 Office and the Chesapeake Bay Program Office need nitrogen deposition and source attribution information to address the atmospheric component of loading of nitrogen to the Chesapeake Bay. Estimates of the airshed affecting the Bay were completed and reviewed.

In FY-1996, a 20-km version of RADM, which more accurately depicts deposition gradients and deposition to the water surfaces of the Bay, was used to estimate the nitrogen deposition reductions possible from ozone-driven regional- and national-nitrogen oxide emission reductions under the 1990 CAAA. These estimates were made available to the Chesapeake Bay Water Quality Model. This work is to provide technical input to discussions in 1997 regarding renewal of the Bay Agreement by the Bay States and EPA. A RADM study was completed during FY-1996 to estimate source region responsibility for the nitrogen deposition to the different water basins of the Bay as part of a cost analysis of air controls relative to their ability to reduce nitrogen load to the Bay (U.S. Environmental Protection Agency, 1996a). This work is being extended in FY-1997 and FY-1998. RADM estimates of source attribution generated in FY-1997 will be used.

2.1.19 ASMD Library Home Page

The ASMD Library developed a world-wide web (WWW) home page (http://www.epa.gov/asmdnerl/library/library.htm), which provides a brief overview of the Library's history and location. The purpose of the home page is to make accessible information about the Library's collection, policies, and services to the Division staff and other users in Research Triangle Park, North Carolina, and other locations. The Library's book and journal collections are cataloged in both the NOAA and EPA library catalogs. Accordingly, the home page provides Telnet and WWW interface connections to the EPA and NOAA on-line catalogs, respectively. In addition, the page provides links to other information resources through the agencies' home pages and to other WWW resources that reflect the Library's collection and staff needs.

2.2 Atmospheric Model Development Branch

The Atmospheric Model Development Branch develops, evaluates, and validates analytical and numerical models that describe the transport, dispersion, transformation, and removal/resuspension of atmospheric pollutants on local, urban, and regional scales. These are comprehensive air quality modeling systems that incorporate state-of-science formulations describing physical and chemical processes.

2.2.1 Models-3 Advanced Air Quality Modeling

2.2.1.1 Models-3 Project

The Models-3 project seeks to develop a community-based comprehensive air quality modeling system that integrates high performance computing capabilities with flexible and explicit process modules that are amenable to modification and revision, and are capable of addressing a wide-range of air quality issues. The Models-3 system integrates not only traditional air quality modules but also the data preprocessing and postprocessing steps into complete and efficient simulation systems (Byun *et al*., 1995a; Ching *et al*., 1995). The specific goals of the Models-3 project are to (1) develop a state-of-the-art air quality modeling system capable of handling multi-pollutant issues (e.g., oxidants, acid deposition, visibility, and particulate matter); (2) provide a standard interface that facilitates interchange of science modules; (3) provide advanced air quality modeling capabilities with the flexibility to operate at a spectrum of spatial scales, including regional, urban, and point source; (4) develop, diagnose, and optimize advanced process formulations for handling multi-scale interactions (e.g., multi-level nesting and adaptive grids), mixed-media issues, and physical and chemical processes; (5) conduct a program of both operational and diagnostic evaluation of the modeling system and its science components; (6) develop and implement advanced approaches to sensitivity and uncertainty analysis; (7) more closely couple meteorological models with chemistry-transport models; (8) take advantage of the enhanced computational capabilities provided by high performance computing and communications (HPCC) architectures; and (9) offer sufficient extensibility to address and fulfill the Agency's anticipated air quality research modeling needs and multi-media regional vulnerability assessments. The science basis and components of Models-3 will be documented in a series of Models-3 science documents.

The project is directly linked to the High Performance Computing and Communication (HPCC) program whose general and specific features are described elsewhere. The Models-3 system is being developed within a high-performance computing technology framework to take advantage of and far surpass the computers and networking capabilities in use. The system will rely on state-of-the-art information processing hardware, software, and networks across many different types of computers: multi-processor vector supercomputers, massively parallel processor (MPP) computers, mainframes, and workstations. The real power of Models-3 will be its ease of use; the complicated system is transparent to the user. The user can build a customized model from the processor library, access data files, run the model, monitor interim results, and perform an interactive graphic rendering of model output in an X-Window environment. Models-3 will be the system to address future policy and scientific questions regarding air quality modeling.

2.2.1.2 Models-3 Science Model Design and Prototypes

Prototypes of the Models-3 air quality model (AQM) serve to test the following science and system concepts: (1) flexibility (the ability to address such multiple air quality issues as regional- and urban-scale oxidant and acid deposition); (2) functional modularity and extensibility (modular and interchangeable science process implementation using a consistent input and output subsystem); (3) systematic and integrated sensitivity and uncertainty analysis; and (4) key algorithms adapted for high-performance computational platforms. The requirements of the initial operating version (IOV) are divided into two categories: (1) the minimum requirements, which specify the minimum acceptable functionality for an operational Models-3 system and the minimum hardware and system software necessary for system development and operation; and (2) the targeted capabilities, which describe the capabilities to be included in the IOV in addition to those on the minimum requirements list (Byun *et al*., 1995a; Dennis *et al*., 1996).

The system framework design paradigm for rapid prototyping is based on object-oriented analysis, which defines object relationships. The framework has multiple processing layers such as the user interface layer, system manager layer, UNIX environment layer, computational program layer, data access layer, and data storage layer. This layered structure helps to update the system components without having to redesign the entire framework when a substantial development has occurred in one or two processing layers (Byun *et al*., 1995b). This is further facilitated by the flow level modularity structure of Models-3. The top level of the system consists of the framework and science models. The second level of modularity consists of the science modeling subsystems, which include the meteorology modeling subsystem, emissions modeling subsystem, chemistry-transport modeling subsystem, and interface processors. The third level of modularity handles the Chemistry Transport Model (CTM) science processes. The CTM maintains different options for science processes such as advection, vertical diffusion, chemical transformation, source addition, pollutant removal process, and cloud processes.

Modularity of the science process is achieved by simplifying module interfaces and minimizing data dependency among the modules. Each science process module encapsulates the computation of a single significant atmospheric process as it affects the concentration field. These modules make the dependencies explicit on the coordinate systems and grid scales; have no sequential data flow dependencies among themselves; and employ a standardized interface to the driver process, promoting interchangeability and extensibility. The data dependency among the process modules are strictly limited to accomplish plug-compatibility and interchangeability modular source codes. This modular concept helps development of plug-compatible processor analysis routines, which is essential to understanding model output. Information from the processor analysis modules will help enhance model parameterizations and algorithms.

The fourth level of modularity defines functional routines within process modules. The distinction of science parameterization algorithms are promoted by numerical solver routines, which allows for easier optimization of different computer architectures. Also, the distinction of I/O (input/output) routines, diagnostic analysis routines, and quality assurance routine is promoted within a science module (Byun *et al*., 1995b).

A key milestone of this project is the integration of science code with the system framework. The key integration tasks are implementation of the science code with the model builder, which helps assembly and compilation of the science code to make an executable program; study planner, which provides a visual mechanism that links science and system processors to produce scientifically useful outputs from the system; program manager, which facilitates registration of executables and scripts; and database manager, which maintains system persistent objects, metadata, and data files.

The IOV of Models-3 includes a linear chemistry model prototype, engineering model prototypes, RADM chemistry prototype, generalized-coordinate and generic grid prototypes, generalized chemistry-solver prototypes, sensitivity algorithm prototypes with automatic differentiation, and multi-level nesting prototypes with generalized coordinates. Also, exploratory model prototypes will be created for a data flow study, an atmospheric transport study, a two-way nesting and adaptive grid study, an uncertainty and sensitivity study, a MPP technology study, and an aerosol and particulate study.

2.2.1.3 Chemical Transport Module Dynamical Processes

In Models-3, the governing equations for the CTM dynamic processes are expressed in terms of the generalized coordinates to facilitate linkage of CTM to many different types of meteorological models. Starting with the tensor algebra, the generalized governing equations were derived for CTM. The generalized CTM can deal with several different conformal map projections as horizontal coordinates and many popular vertical coordinates used in atmospheric modeling studies. Horizontal coordinates supported are Mercator, Lambert, and Polar stereographic projections. Vertical coordinates supported are Sigma-p hydrostatic, Sigma-z, and height. The governing atmospheric diffusion equations include the conservation equation for air, the equation for trace gases, and other diagnostic equations for contra-variant wind components. Vertical mixing is presented with Reynolds flux terms, which can be implemented either using local or non-local closure parameterizations.

In Models-3, advection in CTM is represented in flux form. Advection algorithms implemented are the Bott scheme based on polynomial description of subgrid concentration, Smolarkiewicz iterative upwind scheme, and piecewise parabolic method. Other algorithms being tested are the accurate spatial derivative, and Yamartino-Blackman cubic algorithm. In addition to the flux-form advection algorithms, research is focusing on the treatment of boundary flux, one-way/two-way nesting methods, and multi-level nesting model structure.

The atmospheric mixing process in CTM is represented with Reynolds flux terms. Depending on the atmospheric stability conditions, local and non-local mixing schemes are used in CTM. The vertical mixing algorithms under study are the eddy diffusion (K-Theory), turbulent kinetic energy method, and Asymmetric Convection Model. The results are compared with atmospheric mixing predicted by the transilient turbulence method. The deposition flux as the bottom boundary condition is included in the vertical mixing algorithms available in Models-3. To assess the need for a horizontal diffusion process in CTM, studying the quantification of numerical horizontal diffusion of advection schemes has begun.

2.2.1.4 Aerosol and Visibility Module

A visibility module was developed from the Regional Particulate Model (RPM). The input variables are the aerosol complex index of refraction, the geometric mean diameter, geometric standard deviation, and the total volume of each mode. The integrals of the Mie extinction efficiency over a log-normal size distribution are smooth functions of the geometric mean diameter for a fixed wavelength (Heintzenberg and Baker, 1976; Willeke and Brockmann, 1977). Thus, the extinction coefficient is easily calculated. The algorithm is simple enough to be incorporated directly into the model calculation. The output of the module is the extinction coefficient and the visual index in deciview units (Pitchford and Malm, 1994).

2.2.1.5 Photolysis Rates

An advanced module was developed for specifying photodissociation rates for the Models-3 (Roselle *et al.*, 1996). The module combines advanced radiative transfer models (Madronich, 1987; Zeng *et al.*, 1996) with detailed spatial and temporal data. Photolysis rates are computed for gridded modeling domains by performing hourly radiative transfer calculations on each grid cell using modeled temperature and pressure profiles from MM5, modeled cloud fields, gridded surface albedo, and total ozone column data. The module also offers a generalized framework for specifying different sets of absorption cross section and quantum yield data, to allow generation of photolysis rates for any chemical mechanism (e.g., RADM2, CB4, SAPRC, etc.). The module can perform radiative transfer calculations using either simple two-stream approximations or a more complex multi-stream discrete ordinates method. Development of the module is ongoing, focusing on incorporating satellite cloud data into the radiative transfer calculation and linking the cloud transmissivity and optical properties directly to MM5's calculations. Testing and evaluation will be performed using the Models-3 framework.

2.2.1.6 Aqueous-Phase Chemistry Module

The aqueous-phase chemistry module from RADM (Walcek and Taylor, 1986) was recoded for computational efficiency and readability, and for incorporation into Models-3. In addition, an object-oriented prototype version of this module was developed. This generalized processor was developed as a stand-alone application, but is intended to be integrated with the Models-3 cloud and aerosol modules. The main thrust of the development was to have a self-configuring module with easy access for modification and upgrades of the science. The module uses configuration files that are read in at run time to specify an aqueous chemistry mechanism similar to that done in many gas-phase modules. The method of solution can also be changed in this way without recompiling or restarting the code.

2.2.1.7 Plume-in-Grid Effort for the Models-3 System

Plume-in-grid algorithms were developed to provide a realistic treatment of the subgrid scale physical and chemical processes impacting pollutant species in plumes emitted from major elevated point sources. The key modeling components developed to treat the relevant processes at the proper spatial and temporal scales for pollutant plumes include a Plume Dynamics Model (PDM), which provides the position and physical dimensions of individual plume sections by simulating plume rise, plume vertical/horizontal growth, and plume transport (Godowitch *et al.*, 1995), and a Lagrangian Reactive Plume Module (LRPM), which simulates the relevant processes for a moving array of attached cells representing a plume vertical cross section. LRPM was adapted and incorporated into CTM to simulate the processes governing reactive pollutants for multiple plume sections released from selected major point sources situated within the Eulerian gridded domain. The output parameters from PDM as well as gridded concentration and parameter fields available in CTM will be used to drive LRPM during the subgrid scale phase for each pollutant plume. Testing is underway to identify the physical and chemical criteria for transferring the pollutant plume mass into the grid system at the proper time and location.

In support of this effort, Eulerian grid and Lagrangian simulations were conducted using the Urban Airshed Model (UAM) and LRPM, respectively, to investigate the effects of spatial resolution on pollutant concentrations, particularly secondary species like ozone generated downwind of a point source (Godowitch, 1996). NO_x emissions from a single major point source were simulated in each modeling approach. Using UAM, a range of grid cell sizes from 2 km to 30 km were applied with the same modeling domain. Common inputs were applied in both models to promote a comparison of the results. Preliminary results indicate a broad plume and lower peak ozone downwind of the source for the coarsest grid sizes due to the initial overdilution of the point emissions. With the finer grid sizes of 2 km or 4 km, the evolution of ozone in the plume was captured rather well with the near source ozone deficit recovering and becoming an ozone bulge downwind. Peak ozone concentrations were lower in the LRPM simulations than the peak values obtained from the Eulerian results for any grid size. The prototype plume-in-grid approach will be evaluated as part of the greater Models-3 effort using the Southern Oxidant Study's Nashville 1995 field experimental data.

2.2.1.8 Meteorology-CTM Interface Processor

Meteorology-CTM Interface Processor (MCIP) links output of Mesoscale Meteorology Model Version 5 (MM5) with Models-3 CTM. Its major function is translating output files of MM5 meteorological parameters into the format suitable for CTM operation. Those meteorological parameters not provided by MM5 are estimated using appropriate algorithms in the program. MCIP reads output files from the MM5 and processes meteorological parameters suitable for the CTM simulation. It produces comprehensive meteorological information for the CTM domain. Some of the meteorological data is directly passed through from MM5 parameters, while other parameters are computed using appropriate diagnostic formulas. The output files generated are in the Models-3/EDSS input/ouput applications program interface format.

Although MCIP is not a Models-3 conforming processor, it is designed to be compiled and executed using a configuration file and execution run script similar to a standard Models-3 processor. MCIP uses several Models-3 system persistent objects to interface MM5 data with CTM and other Models-3 science programs. As key processing steps, MCIP:

- Reads MM5 output files for the entire MM5 domain.
- Extracts MM5 output for the CTM window domain.
- Interpolates profile data if output at a horizontal resolution higher than the original MM5 is needed.
- Collapses profile data in vertical direction if output at a vertical resolution is coarser than the original MM5 is needed.
- Computes planetary boundary layer (PBL) parameters and fluxes if needed.
- Computes dry deposition velocities.
- Estimates vertical velocity, density, and model layer heights.
- Estimates cloud characteristics.

2.2.1.9 Postprocessors – Process Analysis

Photochemical simulation models are routinely used to predict ambient concentrations of photochemically produced pollutants and their precursors. Often, predictive performance of the model is assessed by comparing model predictions with measured ambient concentrations. Although such performance assessments are critical in establishing the viability of a model, they provide little insight into the important factors affecting model predictions. Sensitivity analyses are often used to quantify the relative importance of modeled processes, but they too are often unable to adequately characterize important model interactions, especially in highly nonlinear photochemical systems.

Over the past several years, researchers at the University of North Carolina at Chapel Hill, Chapel Hill, North Carolina, have developed diagnostic methods that quantify the relative contributions of the individual model processes, which in turn allow important chemical characteristics of the reacting system to be determined. In their approach, the rate of change in concentration due to each science process (e.g., advection, diffusion, emissions, etc.) and each chemical reaction rate is integrated over a prescribed time period (1-3 hours). These calculated integrated rates provide the total mass throughput for each physical process and each chemical reaction during that period. The throughputs thus provide a direct measure of the relative importance of the science processes. The integrated chemical reaction rates can also be used to elucidate important chemical characteristics of the reacting system, such as the hydroxyl radical and nitric oxide chain lengths. This process analysis method was implemented in the Models-3 prototype system. Since Models-3 is designed to accept alternative chemical mechanisms in a generalized fashion, a special process analysis control program was developed to permit analysts to tailor process analysis to the particular mechanism being employed, and the Models-3 CTM was instrumented to compute the integrated rates requested by the control program. By including process analysis among other diagnostic tools in Models-3, model analysts will be able to better understand the underlying reasons for model predictions. Such information will be particularly important in explaining differences in model predictions that arise from changing model inputs or from changing individual components of the model, such as the chemical mechanism, advection algorithm, etc.

2.2.1.10 Aggregation Tools

As part of the Models-3 framework, the aggregation approach referenced in Section 2.2.3.2 was utilized with the National Meteorological Center (NMC) 700 mb wind data for areas of North America (25°N to 60°N and 50°W to 130°W) to develop cluster patterns from which episodes can be selected. Aerometric data from numerous networks were incorporated. The networks included, but were not limited to, Clean Air Status and Trends NETwork (CASTNET), National Acid Deposition Program (NADP), Interagency Monitoring of PROtected Visual Environments (IMPROVE), and National Dry Deposition Network (NDDN). This will allow the achievement of aggregation for numerous chemical species and visibility.

2.2.2 Photochemical Modeling

The Regional Oxidant Model (ROM) development program started over 12 years ago to provide a scientifically credible basis for simulating the regional transport and collective fate of emissions from all sources over regional scales (1000 km) in the eastern United States; thereby, serving as a basis for developing regional emission control policies for attaining the primary ozone standard in the most cost-effective way. ROM was the first model to be used in comprehensive studies of regional photochemical oxidants. ROM applications provided many useful insights into the rural and urban oxidant interactions in the eastern United States, especially with regard to biogenic hydrocarbon emissions.

The major activity in FY-1996 was the publication of a comprehensive modeling study for the eastern United States, which explored the sensitivity of the photochemical environment to various potential reductions in ozone precursor emissions (Roselle and Schere, 1995). The study compared various combinations of anthropogenic NO_x and VOC emission reductions through a series of ROM simulations. Seventeen simulations were performed with ROM for a 9-day period in July 1988. Across-the-board anthropogenic NO_x and VOC emissions were reduced by different amounts in each simulation. Maximum O_3 concentrations for the period were compared between the simulations. In addition, response surfaces of O_3 and other trace gases to emission reductions were developed. Analysis of the simulation results suggests that (1) most of the eastern United States is No_x limited; (2) areas with large sources of NO_x

are VOC limited; (3) meteorology plays an important role in the buildup of regional O_3 and influences the limiting factor for O_3 formation; and (4) the behavior of other trace gases as predicted by ROM is consistent with the understanding of the chemical system responsible for the buildup of regional scale O_3. FY-1996 was the final year of the ROM program. Subsequent oxidant modeling studies will be conducted with Models-3, which is a third generation modeling system capable of treating oxidants, fine particles, and acid deposition on several scales ranging from urban to regional.

2.2.3 Aerosol Research and Modeling

The objectives of this effort are to develop, evaluate, and refine atmospheric modeling systems that are capable of addressing environmental issues associated with aerosols. These issues incorporate all the known major physical and chemical processes affecting the concentration distribution, chemical composition, and physical characteristics of atmospheric aerosols.

2.2.3.1 Regional Particulate Model

The Regional Particulate Model (RPM) is an expansion of RADM. The effort during FY-1996 centered on two tasks. The first task was to study the effect of sulfur dioxide emission reductions required under the 1990 CAAA. The second task was to transfer the science from RPM (Binkowski and Shankar, 1995) to the Models-3 framework. A preliminary version was developed and modified to make more efficient use of active memory within sub-modules of the aerosol codes.

The 30 meteorological episodes used in the RADM work for the National Acid Precipitation Assessment Program (NAPAP) formed the basis for the study. The 1990 interim emission data set was used for the baseline calculation. A composite emission database for 2010, which included controls for both photochemical oxidant and acidic deposition, was used for the projection of possible beneficial reductions in aerosol particle concentrations and improvements in visibility.

2.2.3.2 Aggregation Research for Fine Particulate Matter

Results from an aggregation method, initially developed for acid-deposition applications, were applied to a limited number (30) of RADM simulations to provide estimates of long-term ambient air concentrations of fine particulate matter (diameter $\leq 2.5\ \mu$). These particles are of increasing concern because epidemiological studies link an increase in mortality and other detrimental health effects to fine particulate matter. The aggregation method is based on the premise that at any given location ambient air concentrations of fine particulate matter are governed by a finite number of different, though recurring, meteorological regimes. If a collection of concentration patterns representative of these different meteorological regimes can be identified, they can be aggregated using appropriate weights to produce reasonable estimates of annual averages.

The 30 original RADM simulation periods proved to be very representative from a fine particulate matter perspective (Eder and LeDuc, 1996a; 1996b). Whereas acid-deposition aggregate values were within 20 percent of the observed values at only 13 of the 20 sites used in the original study, roughly two-thirds (41/64) of the aggregate extinction coefficients were within 5 percent of the mean observed coefficients in the study, and all were within 15 percent. The correlation between the observed and aggregate coefficients was very high and little systematic bias was found in the results. It should be noted that some of the increase in the representation of these 30 simulation periods for particulate concentrations — as opposed to acid wet deposition — can be attributed to the removal of the uncertainty inherently associated with precipitation. Results of this analysis suggest that the original 30 RADM simulations are indeed sufficient to derive annual estimates of fine particulate matter.

2.2.4 Atmospheric Toxic Pollutant Deposition Modeling

Prompted by Congressional mandates, three atmospheric modeling assessments of human exposure to toxic pollutants in the environment are continuing. The first study considers atmospheric mercury exposure from all major anthropogenic sources; the second study handles dioxin-like compounds, and other designated toxic air pollutants specifically from electric power generating utilities; and the third study focuses on exposure to toxic metals.

2.2.4.1 Mercury Modeling

The first study is a cooperative effort with other research laboratories; multi-media model results are provided to the Agency. The REgional Lagrangian Model for Air Pollution (RELMAP) (Eder *et al*., 1986) was previously adapted to simulate the emission, transport, dispersion, atmospheric chemistry, and deposition of mercury across the continental United States. The atmospheric chemistry algorithm, based on formulations of Petersen *et al*. (1995), considers the reaction of elemental mercury with ozone to produce inorganic mercury and the reduction of inorganic mercury to elemental mercury. Model adaptation and testing continued during FY-1996 in response to scientific critiques of model results. Assumptions about the chemical and physical form of the air emissions from various source types were modified to reflect new information from source testing. The updated RELMAP Mercury Model was applied to calculate 1989 monthly mean air concentrations and wet and dry deposition amounts of mercury across 40-km grid cells covering the entire lower 48 States. Division personnel participated with researchers throughout the United States in the interpretation of these results, which were integrated with results obtained for other environmental media. A seven-volume Mercury Study Report to the Congress was drafted. The Report is under final review by the EPA Science Advisory Board.

Preliminary modeling plans were developed for a cooperative modeling study involving the University of Michigan, Ann Arbor, Michigan, and Division personnel. Source sampling and ambient monitoring data collected in south Florida during August and September of 1995 will be used in a three-dimensional Lagrangian model to test various hypotheses regarding atmospheric transformation and deposition processes for mercury, and to assess modeling capabilities for deposition source attribution.

The RELMAP Mercury Model was applied for NorthEast States Coordinated for Air Use Management (NESCAUM) during FY-1996 to simulate concentrations and wet and dry depositions of atmospheric mercury attributable to each source type modeled using updated emission rates for sources within the boundaries of the NESCAUM member states. NESCAUM obtained information previously not available regarding site specific mercury emissions data for medical waste incinerators. For other source types, many of the site specific air emissions data were revised to reflect new process and activity information. Using the previously existing data for non-NESCAUM states and the updated NESCAUM data from the NESCAUM states, RELMAP was applied to estimate a general mass balance of mercury transport to and from the NESCAUM states. This modeling assessment indicated that the majority of atmospheric mercury deposited to the NESCAUM states is emitted from sources outside the NESCAUM region, and that the source types within the region most responsible for intra-regional deposition are related to waste incineration. NESCAUM is continuing to revise the mercury air emissions inventory for its member states, and EPA is revising the nationwide emissions estimates for medical waste incinerators. Further modeling exercises with RELMAP during FY-1997 are planned.

A study was conducted to evaluate the sensitivity of the RELMAP Mercury Model wet deposition results to uncertainty in the chemical and physical form of atmospheric mercury emissions. A single approximation of the fractions of mercury emitted as elemental mercury gas (Hg^0), divalent mercury gas (Hg^{2+}) and particulate mercury (Hg_P) is used for each of the seven major anthropogenic source types modeled. These approximations of the mercury emission speciation are quite uncertain for most source types. Engineering principles suggest that actual emission speciations will vary from source to source based on the composition of the feedstock, the mechanics of the combustion or reaction process used, and the air pollution control technology applied to the exhaust stream. To evaluate model sensitivity, each of the seven major source types was modeled with four emission speciation profiles, (1) the base-case approximation, (2) all Hg^0, (3) all Hg^{2+}, and (4) all Hg_P. Due to the linear chemistry of the RELMAP Mercury Model, the results of the individual source-type simulations could be compiled for each of the 16,384 (4^7) possible combinations and a distribution of possible model outcomes obtained. The distributions of total wet deposition of mercury versus total atmospheric emission of Hg^0, Hg^{2+}, and Hg_P indicated a strong sensitivity of the RELMAP Mercury Model in each case. Based on these results, it was concluded that precise and accurate modeling of atmospheric mercury is dependent on a good understanding of mercury emission speciations and any chemical and/or physical transformations that might take place in the atmosphere after emission (Bullock *et al*., in press).

2.2.4.2 Modeling Dioxin and Other Semi-Volatile Toxics

In the second study, RELMAP was modified and applied to simulate the transport and deposition of 17 separate cogeners of polychlorinated dibenzo-*p*-dioxin and polychlorinated dibenzofuran. This version was used to provide estimates of average annual concentration and wet and dry deposition attributable to the air emissions from electric utility boilers. Human exposure to all dioxin and furan compounds has traditionally been quantified in terms of a summed toxic equivalent (TEQ) to 2,3,7,8-tetrachlorodibenzo-*p*-dioxin, the most toxic of all dioxin/furan congeners. However, the various cogeners of dioxin and furan each have different vapor pressures and gas/particle mass partitioning ratios in the atmosphere. Thus, a scientifically credible treatment of the transport and deposition of total dioxin toxicity required that each congener be modeled explicitly. Once the exposures to each of the 17 congeners was estimated by RELMAP, TEQ was calculated based on prescribed toxic equivalency factors for each congener. The results of this application suggested that some variation does indeed exist in the transport and deposition characteristics of the various dioxin and furan congeners.

To provide the EPA National Center for Environmental Assessment nationwide estimates of exposure to atmospheric dioxin and furan compounds, modifications were made to the RELMAP Dioxin Model to allow the simulation of air emissions from a variety of source types and to incorporate the latest scientific methods for estimating dry gaseous deposition of dioxin and furan compounds to vegetated surfaces. This updated version of the model was used during FY-1996 to assess the average concentration and total wet and dry deposition patterns of 17 known toxic congeners of polychlorinated dibenzo-*p*-dioxin and polychlorinated dibenzofuran over the lower 48 States attributable to air emissions from municipal solid waste and sewage sludge incineration, medical waste incineration, industrial wood- and bark-fired boilers, and coal- and oil-fired electric utility boilers.

The most recently obtained RELMAP dioxin modeling results were presented at a Dioxin Workshop on Deposition and Reservoir Sources held in Washington, D.C., in July 1996. Comments from the expert workshop panel indicated that the model was doing a surprisingly accurate job of simulating the spatial patterns of deposition, given the levels of scientific uncertainty that still exist regarding the semi-volatile behavior of the various dioxin/furan compounds modeled. However, the magnitude of the simulated deposition appeared to be much smaller than experimental monitoring studies would suggest. A closer examination of the dioxin/furan emissions data used by RELMAP revealed that the total mass of the 17 toxic congeners emitted from all sources in the inventory was only about 10 percent of the total mass of all dioxin/furan congeners deposited as measured from monitoring studies. Based on this finding, further development of the anthropogenic emission inventory is planned for FY-1997.

2.2.4.3 Modeling of Heavy Metals

In the third study, RELMAP was modified and applied to simulate the transport and deposition of atmospheric metal particulates such as arsenic, cadmium, and lead. This version was applied to estimate average concentration and deposition patterns for the entire lower 48 States specifically from electric power generating utilities. The results from this simulation were used in the development of a Report to the Congress on Electric Utility Steam Generating Units Hazardous Air Pollutant Study (U.S. Environmental Protection Agency, 1996b). Further applications of this version of RELMAP are planned for FY-1997.

2.2.5 Meteorological Modeling Studies

2.2.5.1 Mesoscale Meteorology Modeling for Air Quality Applications

The Penn State/NCAR Mesoscale Model Generation 5 (MM5) with four-dimensional data-assimilation (FDDA) is to be the primary tool for providing meteorological input data for air quality modeling studies. MM5-FDDA is used with a wide variety of scales and configurations to provide historical, not forecast, meteorology for RADM and Models-3. The model was exercised in one- and two-way nested modes for scales ranging from 108 km to 4 km. Several subgrid convective schemes were used including Kuo, Kain-Fritsch, Grell, and Betts-Miller.

2.2.5.2 Advanced Land-Surface and PBL Modeling in MM5

A new version of MM5 with an advanced land-surface and PBL model was developed to improve surface flux and PBL parameterizations. The model is based on a simple surface energy and moisture parameterization, including explicit representation of soil moisture and vegetative transpiration (Noilhan and Planton, 1989), and the Asymmetric Convective Model (ACM), which was originally developed for RADM (Pleim and Chang, 1992). The coupled surface/PBL model performs integrated simulations of soil temperatures and soil moisture in two layers as well as PBL evolution and vertical transport of heat, moisture, and momentum within the PBL. An important component of the surface model is indirect nudging of soil moisture according to errors in air temperature and humidity predictions compared to analyses of surface observations (Pleim and Xiu, 1995). The version of MM5 incorporating the new surface/PBL model is known as MM5PX.

Evaluation through comparison to field measurements from several experiments have lead to refinements in the stomatal conductance parameterization. The MM5PX results were compared to field measurements of surface fluxes and PBL heights made in the summer of 1994 at Bondville, Illinois, (Pleim *et al.*, 1996). Results of surface fluxes and temperatures from FIFE made in the summer of 1987 in Kansas, and surface flux measurements made in 1995 at Keysburg, Kentucky, will be compared in FY-1997.

2.2.6 Dry Deposition Studies

2.2.6.1 Flux Monitoring Experiments

The Division has developed a mobile flux laboratory (MFL) for directly measuring surface fluxes of O_3, SO_2, CO_2 and HNO_3 (Clarke *et al.*, 1995; Finkelstein *et al.*, 1995). The system also measures the major components of the energy budget as well as those meteorological and vegetation variables required for execution of the Air Resources Laboratory (ARL), Atmospheric Turbulence and Diffusion Division (ATDD) multi-layer inferential dry deposition model. The basic time period of the measurement is 30 minutes except for HNO_3 flux, which is two hours. The objective of the program is to obtain a database for the evaluation and enhancement of dry deposition models (see Sections 2.2.6.2 and 2.2.6.3). Previously, MFL was deployed to measure fluxes above a pasture at Beaufort, North Carolina, during the summer of 1994; above mature corn at Bondville, Illinois, during the late summer and fall of 1994; above a pasture at Sand Mountain, Alabama, during the spring of 1995; and above soybeans at Keysburg, Kentucky, during the summer and early fall of 1995. During 1996, MFL was deployed at Duke Forest, Duke University, Durham, North Carolina; Plymouth, North Carolina; and Rutgers’ Marine Field Station near Tuckerton, New Jersey.

The Duke Forest experiment was conducted from late March through early July in cooperation with Duke University. Profiles of turbulence and trace gas fluxes were measured within and at three levels above the 18-meter loblolly pine canopy. The primary purpose of this experiment was to develop the necessary infrastructure and experience required for the measurement of fluxes above a forest. Analysis of the experimental data will be the focus of the work in 1997.

The Plymouth experiment was conducted within the framework of Project NOVA (Natural emissions of Oxidant precursors: VAlidation of technique) in which university and government scientists cooperated to measure and compare atmospheric eddy correlation flux estimates of surface nitrogen emissions with those obtained from the more traditional chamber studies. The experiment was conducted above a rapidly growing soybean crop from mid-July through mid-August. The experiment measured flux data for O_3, SO_2, CO_2 and HNO_3, and characterization of the energy budget above soybeans.

Flux measurements were made from early September through mid-October. To assess the feasibility of operating the system in a marine environment and to get a preliminary understanding of fluxes to an aquatic system, the instruments were mounted on an existing tower within 5 meters of open water at the Rutgers’ Marine Field Station. These data have not been processed. However, it appears that the system performed well in the marine environment; and the fluxes exhibit much more noise than previously observed over crops due to low concentrations and fluxes, and interference from nearby boat traffic.

2.2.6.2 Inferential Dry Deposition Velocity Model Evaluation

The MFL (see Section 2.2.6.1) measures flux, concentration, and other meteorological variables, and derives deposition velocity (V_d) by dividing the flux by the mean concentration (V_d = flux/concentration). These data are used to assess the magnitude and variability of dry deposition for various land use and meteorological conditions, and to evaluate models of dry deposition processes. The ARL ATDD multi-layer inferential dry deposition model (MLM), which predicts V_d, is being evaluated. The basic time period is 30 minutes for the measured fluxes and inferential model predictions. An initial evaluation was completed of the MLM predictions for three sites: Bondville, Illinois (mature corn), Sand Mountain, Alabama (pasture), and Nashville, Tennessee (soybeans).

Two simple statistical measures are initially used to evaluate the model; mean bias and scatter of the bias. Bias is defined as the observed value (measured) of V_d minus the predicted (model) value (O-P). Scatter, or precision, is the standard deviation of the individual bias observations, $\sigma_{(O-P)}$. Table 1 summarizes the bias and precision, the percent fractional bias and percent fractional precision for O_3, and SO_2 for the three sites. Fractional bias is defined as bias divided by absolute value of the mean observed deposition velocity for that period, and fractional precision as the precision divided by the same mean observed deposition velocity. Results are summarized several ways; for all values, for observations taken during the day, and for night. Day is defined as all half-hour periods beginning between 09:00 and 15:00 LST, while night includes all half-hour periods beginning between 20:00 and 04:00. The transition times (sunrise and sunset) are not included in the day/night comparisons. Note from Table 1 that the bias and precision of the model performance differ considerably between the day and night and between sites. The site differences are reasonably consistent across pollutants and times, implying that model performance is crop dependent and time of day dependent. The fractional biases tend to be about the same for O_3 from day to night for Bondville and Nashville, Tennessee. It is higher during the day than at night for SO_2 for Sand Mountain. The fractional precisions are usually higher than the fractional biases, and in general are higher at night than during the day, indicating that the model performance has considerable scatter, with even more scatter during the night than during the day. Further analyses looking at other statistics and other breakdowns of the data are ongoing. The results are being prepared for a journal article.

2.2.6.3 Dry Deposition Modeling

A new technique for modeling dry deposition of gaseous chemical species was used to take advantage of the more sophisticated surface model implemented in MM5PX. The modified MM5 has a parameterization of evapotranspiration, the same stomatal and canopy conductances can be used to compute dry deposition velocities of gaseous species. This technique has the advantage of using more realistic estimates of these conductances resulting from the integrated surface energy calculation in which the soil moisture is continually adjusted to minimize model errors of temperature and humidity. Other surface resistances needed for the estimation of dry deposition velocity are parameterized according to relative solubility and reactivity in a similar manner to the scheme used in the Acid Deposition and Oxidant Model (ADOM), CALifornia PUFF Model (CALPUFF), and Industrial Source Complex Model - Version 3 (ISC3) (Pleim *et al*., 1984). However, many parameters in this scheme are being updated according to more recent experimental data. Also, an additional deposition pathway through the canopy to the ground was implemented.

The results of the dry deposition model for ozone are being compared to field measurements at Bondville and Keysburg. These results also are being compared to the results of MLM that was used for CASTNET. Preliminary results from the Bondville study were presented by Pleim *et al*. (1996). Results from both studies show better agreement with ozone deposition velocity measurements for the new model than for MLM. This is particularly the case during daytime hours when evapotranspiration is important.

Table 1. Comparison of the multi-layer model predictions of deposition velocity to observations made at three research sites for both ozone and sulfur dioxide

Site	O_3						SO_2					
	All		Day		Night		All		Day		Night	
	Bias FB(%)	Prec. FP(%)	Bias FB(%)	Prec. FP(%)	Bias FB(%)	Prec. FP(%)	Bias FB(%)	Prec. FP(%)	Bias FB(%)	Prec. FP(%)	Bias FB(%)	Prec. FP(%)
Bondville (Corn)	-0.04 -18	±0.15 88	-0.07 -19	±0.21 60	-0.04 -27	±0.18 81	-0.11 -24	±0.40 85	-0.25 -37	±0.60 89	-0.01 -3	±0.23 71
Sand Mt (Grass)	0.02 7	±0.16 67	0.04 11	±0.19 46	-0.04 -35	±0.09 88	-0.12 -20	±0.36 62	-0.19 -24	±0.37 49	-0.08 -21	±0.32 90
Nashville (Soy Beans)	-0.13 -36	±0.25 66	-0.21 -36	±0.26 43	-0.05 -33	±0.18 127	-0.38 -46	±0.52 63	-0.50 -49	±0.51 51	0.03 14	±0.29 133

2.2.7 Technical Support

2.2.7.1 North American Research Strategy for Tropospheric Ozone

The North American Research Strategy for Tropospheric Ozone (NARSTO) is a plan for a coordinated 10-year research strategy to pursue the science-based issues that will lead to better management of the North American tropospheric ozone problems. It includes a management plan for performing this coordination across the public and private sector organizations sponsoring ozone research, as well as those groups performing the research, including the university community. Canada and Mexico also are participating in the continental NARSTO plan. During FY-1996, two Division representatives were involved in co-chairing key teams for the continental NARSTO program: the modeling team and the analysis and assessment team. Also, the first major activity of NARSTO began, a state-of-science assessment for tropospheric ozone. The assessment will be composed of a series of critical review papers on particular areas of the science, as well as a report on how science can address outstanding policy issues in tropospheric ozone. The critical review papers and assessment report are due to be published by the end of 1998. Within the Agency, all non-effects scientific aspects of tropospheric ozone research, including atmospheric chemistry, modeling, monitoring and field studies, methods development, emissions research, and emissions control technology are being coordinated and managed by a Division member, as part of the EPA contribution to NARSTO.

2.2.7.2 NARSTO-Northeast

A major field study was begun during the summer of 1995 to collect data in the northeast United States to provide new insights into the photochemical ozone problem, including regional transport of ozone and its precursors. Additional surface monitoring stations were set up to measure ozone, nitrogen oxides, and hydrocarbons upwind and far downwind of the major East Coast urban areas. These stations supplement the data of the existing EPA/State Photochemical Assessment Monitoring Stations (PAMS) in the urban areas. In addition, the meteorological network in the Northeast was augmented during the study with additional rawinsonde releases and the deployment of several radar profilers with RASS systems.

Two aircraft were also used to obtain measurements aloft during ozone episode conditions. The analysis and modeling components of the study began during FY-1996. The study is expected to continue through 1997. Resources for NARSTO-NE derive from both public and private sources, with the utility industry providing funds for the non-PAMS measurements and EPA and the States providing PAMS support. One Division member represents EPA/ORD on the NARSTO-NE Executive Steering Committee and also serves as chair of the Data Management Committee.

2.2.7.3 Cooperative Regional Model Evaluation Project

The Cooperative REgional Model Evaluation (CREME) project was initiated during FY-1993. It involves applying ROM, UAM (Versions IV and V), and the SARMAP Air Quality Model to the 1991 Lake Michigan Ozone Study (LMOS) database, and the 1988 northeast United States database. The American Petroleum Institute, Electric Power Research Institute, and Coordinating Research Council are sponsoring the project to apply and evaluate these contemporary regional and urban-scale photochemical grid models to the intensive field databases. One Division representative is on the Steering Committee. Both model evaluations and diagnostic/sensitivity analyses are being performed. During FY-1996, model simulations were conducted for the northeast United States, using the UAM IV and V in various configurations.

Results showed that there were no significant improvements in performance evaluation for ozone of one model over the other. When comparing upwind ozone boundary conditions for the urban modeling obtained from both ROM and UAM-V simulations, ROM was seen to overpredict because of a bias in the wind directions. Work began on applying the SARMAP Air Quality Model (SAQM) to the northeast United States.

2.2.7.4 Southern Oxidant Study

FY-1996 was the sixth year of the multi-year Southern Oxidant Study (SOS), a major field and modeling project concerned with the generation and control of ozone and photochemical processes in the southeastern United States. A consortium of Southeastern universities is coordinating the study. Division personnel are involved in providing technical leadership on aspects of air quality simulation modeling and emission inventory development on various cooperative agreements. The focus of activities within SOS during the past year was on reducing and quality assuring the data obtained from a major field study in and around Nashville, Tennessee, during the summer of 1995. The principal objective was to study the physical and chemical interaction of power plant plumes and the Nashville urban plume with the regional environment. Besides the intensive measurements obtained at the surface, observations aloft were made by several aircraft, including the NOAA Twin Otter and NOAA P3. A preliminary data analysis workshop was held during May 1996. Initial results showed several stagnation events had occurred in the Nashville area during the field campaign. Ozone episodes in the Nashville area were a part of a larger pattern of elevated ozone concentrations in the eastern United States during the period of the campaign. Large gradients in ozone were observed both horizontally and vertically in the Nashville study.

A relational database was developed for the archival and retrieval of air quality, meteorological, emissions, and miscellaneous data collected as part of SOS. The database will house surface, tower, tethersonde, and aircraft measurements collected during regional- and urban-intensives and from regional-surface ozone and intermediate-chemistry networks. In addition, gridded data of typical summer-time emissions were included in the database.

2.2.7.5 Interagency Work Group on Air Quality Modeling

The Interagency Work Group on Air Quality Modeling (IWAQM) was formed in FY-1991 through a Memorandum of Understanding between the EPA, the U.S. Forest Service, the U.S. Fish and Wildlife Service, and the National Parks Service. IWAQM seeks to develop the modeling tools needed to conduct assessments of individual and cumulative impacts of existing and proposed sources of air pollution on local and regional scales with special emphasis on the protection of Class I areas as defined by the CAA. In FY-1996, a comparable data set for a second year (1992) was begun using MM5-FDDA. The goal is to obtain, as a minimum, a three-year database of modeled meteorology fields making possible the implementing of IWAQM recommendation of performing assessments of source impact to Class I areas using local- and regional-scale dispersion models.

2.2.7.6 Federal Advisory Committee Act Subcommittee on Ozone, Particulate Matter, and Regional Haze

New air quality standards for ozone and fine particulate matter are expected to be promulgated in 1997. The EPA is considering a joint implementation of the new standards considering the interactions between ozone and fine particulate matter. To facilitate this implementation, a Federal Advisory Committee Act (FACA) Subcommittee was established to help the EPA in developing guidelines and procedures. Several working groups were established to assist the Subcommittee, including a Base Programs group, Regional Strategies group, Science and Technical Support group, an Integration group, and a Communications group. One Division member is assisting the Science and Technical Support group in developing a conceptual model of the science underpinning the implementation. Comments are also being prepared on the proposed use of scientific methods and tools advocated in policy-oriented issue papers being written by the other working groups.

2.2.7.7 Stratospheric Ozone

The global distribution of total column ozone continues to attract great international attention as concerns over reduced ozone abundances escalate. The spatial and temporal distribution of ozone is poorly understood. To assess anthropogenic changes to date and to better understand how ozone abundance may respond to future perturbations requires a better understanding of its natural intra- and inter-annual variability and the processes that contribute to this variability. Accordingly, the purpose of this analysis is to develop a better understanding of these natural variations across all spatial and temporal scales.

This is being achieved through a new application of rotated principal component analysis and spectral density analysis to a newly released version (Version 7.0) of the total column ozone data derived from TOMS (Total Ozone Mapping Spectrometer) for the extended period of 1980 through 1995. The main objective of this study is to identify, through a reduction in data, the characteristic, recurring, and independent modes of variation across all potential spatial and temporal scales. This technique is ideal for application to the TOMS data set where the total number of observations exceeds 10 million (Eder, 1994).

2.2.7.8 Climatological and Regional Analyses of Clean Air Status and Trends Network Data

The Clean Air Status and Trends NETwork (CASTNET) monitoring program is being evaluated to determine the extent to which cost savings can be achieved while preserving the quality of information provided by the network. As part of this evaluation, rotated principal component analysis was applied to regionalize the CASTNET stations into influence regimes or subregions whose fluxes, concentrations, and deposition velocities exhibit statistically unique, homogeneous characteristics in response to a commonality of forcing factors (e.g., meteorology, emissions, geography). This approach has been used successfully in the examination of other aerometric data, including $SO_4^=$ concentrations in precipitation (Eder, 1989) and ambient air concentrations of O_3 (Eder *et al*., 1993).

Utilization of this technique permitted prioritization of the CASTNET stations in terms of total variance explained; and hence, determine those stations that are most representative and should therefore be retained. A total of 15 stations were found to be most representative. With only a few exceptions, the spacing between recommended stations is rather uniform and fairly representative of the CASTNET domain.

2.2.7.9 Statistical Modeling of Urban Ozone

A two-stage statistical clustering approach designed by Eder *et al*. (1994) for Birmingham, Alabama, was applied to Houston, Texas, in an effort to refine the approach and simultaneously account for the variability observed in ozone attributable to meteorology in the Houston area. Refinements included replacing principal component analysis with singular value decomposition, which was used to define the meteorological clusters and the use of non-linear regression as opposed to linear regression, which was used to provide a more realistic model. Results indicated that a one-stage clustering approach utilizing hierarchical clustering alone performed better when compared with a two-stage approach involving average linkage and hierarchical clustering.

2.3 Fluid Modeling Branch

The Fluid Modeling Branch conducts laboratory simulations of atmospheric flow and pollutant dispersion in and around complex terrain and other obstacles and in the convective boundary layer; dense-gas plumes; and pollutant dispersion in other complex flow situations that are not easily handled by mathematical models. The Branch operates the Fluid Modeling Facility, consisting of large and small wind tunnels, a large water channel/towing tank, and a convection tank. The large wind tunnel has an overall length of 38 m with a test section 18.3 m long, 3.7 m wide, and 2.1 m high. It has an airflow speed range of 0.5 to 10 m/s, and is generally used for simulating transport and dispersion in the neutral atmospheric boundary layer. The towing tank has an overall length of 35 m with a test section 25 m long, 2.4 m wide, and 1.2 m deep. It has a speed range of 0.1 to 1 m/s, and the towing carriage has a range of 1 to 50 cm/s. The towing tank is primarily used for simulation of strongly stable flow; salt water of variable concentration is used to establish density gradients in the tank, which simulates the nighttime temperature gradient in the atmosphere. A convection tank measuring 1.2 m on each side and containing water to a depth of 0.4 m is used to study the convective boundary layer (CBL), and flow and dispersion under convective conditions. The tank is temperature stratified using an electrical heating grid, then convection is initiated by heating the floor of the tank. This produces a simulated convective boundary layer capped by an overlying inversion. Another activity of the branch is the study of resuspension mechanics and wind erosion, primarily through experimental field measurements.

2.3.1 Plume Penetration of Elevated Inversions

The penetration of buoyant plumes into an elevated inversion above the convective boundary layer was investigated using the convection tank. This completed a lengthy effort to develop the convection tank facility and laser-induced-fluorescence measurement technique. Specific components of the system include (1) a laser light-sheet generation system using a computer-controlled galvanometer and a parabolic reflector, (2) a video camera synchronized to the laser scanner, and capable of high-speed video acquisition and disk storage, (3) a mechanical system linking the video camera and laser system that eliminates distortion by maintaining a constant optical path length between the laser light sheet and the camera, (4) a motion-control system that traverses the laser light-sheet system at specified speed and acceleration, (5) a motion-control system that traverses a source of dye through the tank, and (6) sensors, actuators, and software that synchronizes all systems and monitors all critical timing and positioning. In addition to these primary systems, other systems automatically stratify the water in the tank using an electrically-heated grid, start and stop the source dye, initiate convection by electrically heating the floor of the tank, and cool and filter the water between experiments to allow several experiments to be performed each day. Specialized software was also developed to analyze the resulting video frames, correct for optical aberrations, and attenuate and convert video intensity levels to dye concentration through a system calibration curve.

Buoyant plumes were simulated in the tank by using a mixture of water, methyl alcohol, and fluorescent dye. These plumes were released from a source that was towed across the tank near the floor. The tank was initially stratified to produce an elevated inversion similar to that which typically exists above the fair-weather CBL. Convection was then initiated by heating the floor of the tank with electrical heaters. Plume cross sections were sampled at fixed distances downstream of the source by illuminating a slice of the plume with a sheet of light from an argon-ion laser. The laser light induced fluorescence in the plume in proportion to the dye concentration. The resulting fluorescence was recorded by a video camera and subsequently converted to dye concentration.

Because the tank is of limited size, measurements at a fixed distance downstream of the source can only be made for a short duration, and an ensemble of experiments is typically required in order to obtain stable plume statistics. Automation of the entire measurement process allowed an ensemble to be measured under as near identical conditions as possible.

Figure 1 summarizes the experimental results obtained from ensembles of results at eight downstream distances and for plumes, which were neutrally buoyant ($F^*=0$), weakly buoyant ($F^*=0.1$), moderately buoyant ($F^*=0.2$) and strongly buoyant ($F^*=0.4$). The vigorous mixing due to large-scale convection is evident in all cross sections. Plumes released near the floor of the tank are quickly dispersed through the depth of the CBL. As the plume buoyancy increases, the plume rises to the base of the overlying inversion, subsequently being brought to the surface through fumigation. For the most highly buoyant plumes, the plume clearly penetrates into the overlying inversion, spreading broadly and reducing the effectiveness with which the turbulence in the CBL entrains plume material and mixes it to the surface; much of the plume remains aloft. Statistics describing these plume penetration experiments are being used to develop new models for prediction of dispersion processes in the convective boundary layer.

2.3.2 Dense Gas Dispersion

Three projects were completed as part of a continuing investigation into the behavior of dense-gas plumes. The first of these was preparation of a data report and thesis (Zhu, 1995; 1996) on a study of dense-gas releases from a small area source within large roughness elements. The second study was instigated through discussions within the Scientific Advisory Committee of the Petroleum Environmental Research Forum (PERF) dispersion modeling project to obtain some information on the vertical entrainment rates within dense-gas plumes over relatively large surface roughnesses and under stable, light-wind conditions. This study is of particular significance because two other wind-tunnel facilities will be conducting identical or similar measurements; this comparison will serve as a test of the general reliability of wind-tunnel testing of ultra low-speed, dense-gas flows. The third study in this series was spawned from earlier studies and was designed to examine intermittency in dense-gas plumes.

Previous dense-gas studies showed that a vertically thin but horizontally wide layer of dense gas (a "vapor blanket") could be formed close to the surface when a large quantity of dense gas was released at ground level. The first wind tunnel study in this series was performed to investigate how this vapor blanket could affect the mean flow and structure of the turbulence in a neutral boundary layer. Special consideration was given to making accurate velocity measurements within the dense-gas plume due to the sensitivity of hot-film (wire) anemometers to the dense gas (carbon dioxide) concentration. The results of the experiments showed that, in the presence of the dense-gas plume, the mean velocity profiles were changed significantly in shape near the surface at low wind speeds. Significant reductions in roughness lengths and friction velocities were also observed. Both the longitudinal and vertical intensities of the turbulence were found greatly

Figure 1. Plume cross sections at various non-dimensional downstream distances (X) from a continuous source emitted into a simulated convective boundary layer with an overlying inversion. F* is a non-dimensional buoyancy.

reduced in the presence of the dense-gas plume at low-wind speeds. These changes and reductions were not only related to the magnitude of the dense-gas concentration, but also to the vertical extent of the dense-gas plume. The gradient Richardson number was shown to be the most appropriate parameter for describing changes in the mean flow and structure of the turbulence.

The second dense-gas study was designed to obtain some information on the vertical entrainment rates within dense-gas plumes over relatively large surface roughnesses under light-wind conditions. It is generally believed that when the plume depth is larger than the roughness element height, the roughness effects may be parameterized through a single variable, the roughness length. However, when the elements are the same height or larger than the plume depth, entrainment will be affected by the shapes, sizes, and spacings of the individual elements. The basic purpose of these experiments was to determine how vertical dense-gas diffusion is affected by different roughness heights, contrasting cases where the plume depth was much smaller than the roughness height with one where it was much larger. These experiments used crosswind line sources at ground level and, through the use of two-dimensionality and mass conservation, it was shown that the entrainment rate could be determined from measurement of the longitudinal surface concentration. This entrainment velocity was determined as a function of the Richardson number. The neutral plume values of entrainment velocity were found to be quite consistent, but somewhat higher than values published in the literature. In general, all the data collapsed into a single curve (Figure 2). The breakpoint of the curve, around a Richardson number of 2, and the slope of the curve above that point, were in general agreement with published literature. Entrainment velocities at the higher Richardson numbers seemed to show effects of laminarization of the plume (molecular diffusion).

The third dense-gas study in this series examined flow laminarization in two-dimensional dense gas plumes. The plume was simulated by releasing carbon dioxide through a ground-level line source into a turbulent boundary layer with an aerodynamically rough surface. Flow visualization revealed that, with increasing Richardson number, both the plume depth and vertical mixing were significantly suppressed, while upstream propagation of the plume from the source was enhanced. The most important feature of the flow revealed by visualization was the plume laminarization which appeared to be closely related to the Richardson number and the roughness Reynolds number. Quantitative measurements within the dense gas plumes showed that the mean velocity and intensity of the turbulence were significantly reduced near the surface, and that these reductions depended systematically on the Richardson number. Application of an intermittency analysis technique confirmed the general flow pattern within the dense gas plume and demonstrated the changes of flow regime with variations in Richardson number and roughness Reynolds number. Based on the intermittency analysis, simple criteria were developed for determining where plume laminarization would occur.

2.3.3 Open Burning and Detonation

The fluid modeling study of the rise through the atmosphere of buoyant thermals produced by open detonation continued this year. This study is being performed in conjunction with the Strategic Environmental Research and Development Program (SERDP) in support of the efforts to develop a mathematical dispersion model for evaluating EPA permit requests to allow larger amounts of material per detonation. The U.S. Government has over 400,000 tons of munitions to be destroyed and open detonation was determined to be the best method of disposal. This laboratory study will provide a database and empirical formulations for inclusion in the dispersion model.

Figure 2. Variation of non-dimensional entrainment velocity with Richardson number.

To simulate the rise of a buoyant thermal, a dense mixture of salt water and blue dye is released instantaneously at the surface of a water tank in the laboratory. As this mixture falls through the water, it is governed by the same equations as a rising thermal in the atmosphere. Last year's efforts were directed at determining a predictive formula for the fraction of a thermal that penetrates a step change in density. During the year, the rise into an elevated linear gradient was investigated. The maximum penetration height, the equilibrium height, and equilibrium thickness of the thermal were found for several combinations of initial thermal buoyancy, height of the base of the inversion, and magnitude of the gradient of the inversion. The maximum height was determined by visual observation. Soon after each thermal approached its equilibrium position, a sample rake with a 10 X 10 array of ports was towed through it collecting line-integrated dye samples. The dye concentration in each sample was measured with a colorimeter and used to compute the height of the center of mass and the vertical thickness of the thermal at its equilibrium position. Two data reports were prepared (Thompson and Snyder, 1996a; Thompson and Snyder, 1996b).

2.3.4 Investigation of Resuspension Mechanics and Wind Erosion

During FY-1996, two field trips and a three-month visit to the University of Paris were the principal activities. The two field trips were a one-month investigation of PM_{10} dust at Owens Lake, California, and a two-week portable wind-tunnel investigation near Las Cruces, New Mexico, on the threshold wind friction velocities for arid and semi-arid soils. The three-month visit to the University of Paris, Paris, France, took place in summer 1996.

The main goal of the Owens Lake experiment was to measure the total PM_{10} dust flux emitted in dust storms on the floor of the (dry) Lake and to measure size distributions of the emitted dust. These measurements are to be related to soil and meteorological conditions in the lake-floor source area. Support for the experiment also came from the Great Basin Unified Air Pollution Control District. Air Resources Laboratory (ARL) Special Operations and Research Division (SORD) provided forecasts of wind conditions at Owens Lake for the month of March.

Erection of meteorological towers and other experimental setups took place March 1-5, 1996. The main experiment took place March 6-26, 1996, during which period data were obtained for five dust storms. The data included more than 200 size distribution samples of dust emitted from Owens Lake. Dismantling, packing, and shipping of the equipment was done March 27-30, 1996.

A field trip in May 1996 had the purpose of measuring the threshold friction velocities and aerodynamic roughness heights of soils located on the Jornada del Muerto Experimental Range. The measurements were done using the NOAA portable wind tunnel. The measurements will be used in a component of a model for dust production and wind erosion of vegetated and non-vegetated soil in the western part of the United States. The measurements were analyzed later in the summer.

A Division scientist visited the Labortoire Interuniversitaire des Systemes Atmospheriques (LISA) for the period June 15-September 12, 1996. The purpose of the visit was to interact with the group modeling dust emissions and the group measuring dust emissions at the University of Paris 12. The primary objective of the visit was to develop common interests with emphasis on the modeling of dust emissions from arid and semi-arid lands. The accomplishments of the visit were:

- Studying the effect of airborne sand grains on the increase in the momentum flux of the wind by equivalently increasing the aerodynamic roughness height. A theoretical treatment of the increase of roughness height was verified and a parameterization was developed that can be used for erosion models.

- Examining the threshold friction velocities and aerodynamic roughness height for a large variety of soils typical of semi-arid and arid areas of the western United States. The threshold friction velocities for undisturbed loose soils and all disturbed soils could be explained by the omnipresence of 60-120 micrometer particles in the tested soils and the effects of stress partitioning on fixed, non-erodible particles present on the soils. The threshold for crustal breakage could be expressed as a function of roughness and of the equivalent size of the individual cracked pieces of the soil crust, where the size expressed a dimension that gave the same volume of crustal pieces. Cyanobacterial lichen soil crusting increases the threshold friction velocity by both creating a rougher surface and by forming larger aggregates that require larger wind stresses to move (Marticorena *et al.*, accepted for publication).

A visit was made to the field experiment, WELSONS (Wind Erosion and Loss of SOil Nutrients in semi-arid Spain), August 12-19, 1996. This was a multinational experiment near Zaragoza, Spain. There were investigators from France, Spain, the Netherlands, and Germany measuring the vertical fluxes of dust, horizontal fluxes of sand, micrometeorology, and soil physical and chemical properties.

2.4 Modeling Systems Analysis Branch

The Modeling Systems Analysis Branch supports the Division by providing routine and high performance computing support needed in the development, evaluation, and application of environmental models. The Branch is the focal point for modeling software design and systems analysis in compliance with stated Agency requirements of quality control and assurance, and for conducting research in the High Performance Computing and Communications (HPCC) program, which includes parallel processing, visualization, and advanced networking. Under the HPCC program, the Branch is developing a flexible environmental modeling and decision support tool to deal with multiple scales and multiple pollutants simultaneously; thus, facilitating a more comprehensive and cost-effective approach to related single- and multi-stressor human and ecosystem problems.

2.4.1 Models-3 Framework/High Performance Computing and Communications

The HPCC program is a cross-agency coordinated program under the leadership of the National Science and Technology Council (NSTC) Committee on Computing, Information, and Communications, which conducts long-term research and development in advanced computing, communications, and information technologies and applies those technologies to achieve Agency missions. The Agency is moving toward community-based environmental management involving stakeholders, local industry, state and local governments, and people in the community whose health, environment, and jobs are most impacted. The primary goal of the HPCC program is to improve the stakeholders capability to access data, reliable environmental models, and visualization and analysis tools to make informed decisions involving risks to human health, ecosystems, and the economics of local industry and surrounding community. This goal is also consistent and supportive of the goals and objectives of the NSTC Committee on Environment and Natural Resources. The HPCC technology research focuses on three areas: environmental assessment framework development; high performance numerical methods for scalable parallel architectures; and public data access and visualization and analysis techniques.

In 1996, the HPCC program continued work on the first version of Models-3, a flexible software system designed to facilitate the development and use of environmental assessment and decision support tools. The initial version of Models-3 focuses on urban to regional scale air quality simulation of ground-level ozone, acid deposition, visibility, and fine particulates. The Models-3 framework provides interfaces between the user and operational models, between the scientist and developing models, and between the hardware and software. This enhances the user's ability to perform environmental management tasks ranging from regulatory and policy analysis to understanding the interactions of atmospheric chemistry and physics, while rapidly adapting to emerging technology. Models-3 is intended to serve as a community framework for continual advancement of environmental assessment tools.

To adapt to changing hardware and software, the framework uses specialized object libraries and a standardized interface design that isolates critical system components. This minimizes the impact of hardware and software upgrades. A client-server architecture, in conjunction with a standardized data interface and object-oriented database containing metadata, enables transparent use of multiple computing platforms and access of data across the network. The object-oriented database contains such shared data as model domain, map projections, grid resolution, and chemical species that enable the interchange of science codes while maintaining user control of the specifics of a model application. A library-based graphical user interface facilitates ease of use for model executions and access to a variety of visualization and analysis packages. Components of Models-3 assist in design and preparation of source emission inventories compatible with a variety of air quality modeling capabilities. A preliminary demonstration of an early Models-3 prototype was held for client office personnel to obtain feedback on its usefulness for the regulatory community. The feedback was very positive.

A Program Control Processor (PCP) was developed for Models-3 that allows a regulatory user to select from existing gas-phase chemistry mechanisms and a model developer to easily modify chemistry mechanisms and corresponding species linkages, without coding changes, to study the effects of different chemical mechanism approaches. PCP can also be used for any of the Models-3 preprocessors that require chemical species or reactions control; and therefore, PCP provides a method of generalizing the chemical mechanism used in the modeling system. In addition, computer memory usage is conserved because the exact species dimensions of the internal arrays in the code are determined at compile time.

2.4.2 Models-3 Extension for Cross-Media Modeling

The primary purpose of this research is to facilitate the development of a community environmental modeling framework to serve as a foundation upon which the scientific and technical communities can build, component by component, complex multi-discipline, and multi-pollutant assessment tools. This effort depends upon emerging technology that enables federal agencies, academia, and research institutions to participate in a collaborative approach to multi-discipline environmental modeling. To test the feasibility of this approach, three models were linked into Models-3 and data conversions were performed to facilitate the exchange of data among the models. The models were RADM for atmospheric deposition, the Hydrological Simulation Program - FORTRAN model for Chesapeake Bay nutrient flow in the watershed to the Bay, and the Chesapeake Bay Water Quality Model with its embedded hydrodynamic model for the Bay response to nutrient loading.

2.4.3 Models-3 Emission Data Processing

The emission data processing module of the Models-3 system was substantially improved, expanded, and renamed during FY-1996. The module is based upon the Geocoded Emission Modeling and Projection (GEMAP) system, now known as Emission Modeling System-95 (EMS-95) (Wilkinson *et al*., 1994).

However, the emission processing module development has resulted in many changes to GEMAP, and the design and development of several emission processing functionalities external to the former GEMAP. Consequently, the new system is now named the Models-3 Emission Processing and Projection System (MEPPS). The principal MEPPS developments included:

- Installing and debugging the U.S. EPA Mobile 5a (U.S. Environmental Protection Agency, 1994), a standard regulatory mobile source emission estimation model. There will be a minor upgrade within MEPPS during the next fiscal year.

- Adding the capability for the user to interactively specify the definitions of very large (major elevated point source emissions), major and minor point sources with a variety of stack-related parameters. This ability is important in defining different emission scenarios for scientific and regulatory modeling analyses.

- Linking the meteorological processor MM5 (Grell *et al.*, 1993) and the CTM module of Models-3. MM5 provides spatially gridded meteorological data to MEPPS and the CTM module in the necessary format (Net CDF I/O API) through a meteorology-chemical interface processor. MEPPS uses temperature and solar radiation data to estimate biogenic and mobile source emissions. MEPPS then provides the emission data in Net CDF I/O API format to the CTM module and associated plume dynamics model.

- Developing and improving user interface screens for each portion of MEPPS to guide the user stepwise through the emission processing system, including the input, output, and spatial and temporal allocation functions. A basic help menu is included.

- Adding automated quality control checking and associated reports, particularly for raw emission inventories, and for the MEPPS output data.

- Developing and testing a suite of geographic information system visualization functions specific to emission inventory data processing and analysis. For example, emission data may be viewed, isolated, identified, and subsets created on-screen.

- Completing an initial draft of a stand-alone general data input processor for Models-3, called the Models-3 Input Data Processor (MIDPRO). Data imported into Models-3 are likely to be in many different formats and of varying degrees of quality. This is particularly true of emission inventory data. However, data from monitoring studies, satellites observations, etc., also will be imported. The MIDPRO will be designed to flexibly import any specified format, automatically perform substantial quality control, and convert the data to internal formats including Net CDF I/O API, ASCII, and SAS. Units will be converted as a part of the import process.

2.4.4 Visualization and Analysis Tools

The primary goal of the visualization and analysis effort is to provide a desktop accessible integrated software system that assists federal, state, and industrial groups in performing environmental research, modeling, assessment, and decision making activities. Two independently developed visualization capabilities were integrated into the Models-3 framework. MCNC in Research Triangle Park, North Carolina, developed the Package for Analysis and Visualization of Environmental Data. It is a flexible, fast, distributed application to visualize multi-variate gridded environmental data sets. Key features include baseline two-dimensional graphics such as x-y, scatter, time-series plots, contours and color mesh plots, access and manipulation of data sets located on remote machines, and support for multiple simultaneous visualizations. Vis5D, a public domain interactive 3-D visualization package developed at the University of Wisconsin, Madison, Wisconsin, provides fast volume rendering of 3-D temporally varying model simulations, projection of values of another variable onto an isosurface, slicing, moving slice, and rotation. Images of clouds detected by the visible and infrared sensors on the Geostationary Operational Environmental Satellite (GOES) were incorporated into Vis5D and overlaid with clouds and meteorological information simulated by MM5 predictions to evaluate how well MM5 simulated clouds compared to real data. A video, *Comparing Model Predictions to Satellite Data*, was produced to demonstrate this tool.

Models-3 also allows the user to visually explore the relationship of measured air concentration data from aircraft flights with surrounding air quality model predicted chemical concentration data. The user is able to view aircraft measurements and model predictions together in time and space along the entire aircraft flight path and the traditional time series graph that compares concentrations in time without regard to spatial location. IBM visualization data explorer routines were developed to allow the user to dynamically display the quantitative photochemical relationships involved in ozone production at each model grid cell and each time step as synthesized from integrated reaction rate and mass balance diagnostics performed by instrumented air quality models. Analysis of these data has led to the discovery of more powerful measurement-based indicators for balancing NO_x and VOC controls for more effective ozone reduction strategies.

2.4.5 Technology Transfer

A cooperative agreement was awarded to conduct research to facilitate the transfer of advanced air quality models planned for inclusion in Models-3. This included using the World-Wide Web on which courses and tutorials were made available during FY-1996: Fabric Filtration Systems (http://www-epin.ies.ncsu.edu/olfabric/homepage.htm); Air Quality Meteorology (http://www.shodor.org/metweb/); and, Computation Atmospheric Chemistry (http://www.shodor.org/cas/).

Two workshops were broadcast by satellite from North Carolina State University, Raleigh, North Carolina, through the Air Pollution Distance Learning Network and are available on videotape: April 23, 1996, *Emissions Modeling and Visualization Tool - Current and Future*; and July 9-10, 1996, *Computational Atmospheric Science: Preparing for Models-3.* Strategy development tools were investigated and three tools tried: genetic algorithm for optimizing multi-objective optimization; modeling to generate alternatives; and automatic differentiation of FORTRAN (Hildebrant, 1996; Loughlin *et al.*, 1996).

2.4.6 Model Developments on Scalable Parallel Architectures

A parallel version of RADM was implemented on the Cray T3D using a one-dimensional decomposition of the chemistry and advection routines. RADM uses operator splitting to decouple the linear and non-linear processes, thus the chemical reaction equations are spatially independent and highly suited to parallel solution. The horizontal transport equations, however, use pollutant concentrations in the neighboring grid cells, which tend to slow computation because of inter-cell communications. The parallel version of RADM was instrumented to output integrated chemical reaction rates and intermediate species (10GB per 5-day model execution). This data is being analyzed to determine measurable chemical indicators for relative effectiveness of NO_x versus VOC emission controls for ozone attainment.

A parallel version of the Models-3 CTM was developed for the Cray T3D and performance was improved using simple grid/block/scattering load distribution and large file buffers for parallel I/O. A portable message passing interface tool was used to move the data between the processing elements (PEs). A FORTRAN dynamic memory allocation method was implemented to enable the use of a variable number of PEs without the necessity of recoding and recompiling for each different architecture configuration. MM5 was ported to the Cray T3D and modified to incorporate FDDA. Work is underway to integrate a new surface flux and planetary boundary layer model (Pleim and Xiu, 1995) into the parallel version of MM5. A new parallel algorithm for solving transport equations using non-uniform rational B-splines was also developed. Computational efficiency gained by using these techniques enable a one atmosphere simulation of a large number of control and abatement options to be evaluated in time frames required by the CAAA.

Significant progress was made via HPCC cooperative agreements in developing high performance computing techniques for sediment modeling and analytical element modeling of groundwater. Researchers at the University of California at Santa Barbara, Santa Barbara, California, developed numerical models of flux, transport, and fate of sediments and associated hydrophobic contaminants in surface waters and conducted modeling studies in the Lower Saginaw River in Michigan and Green Bay in Lake Huron. Researchers at the University of Minnesota, Minneapolis, Minnesota, developed new procedures for incorporating time dependent water density distributions into groundwater flow models for coastal aquifers in response to changing salinity. Researchers at Indiana University, Bloomington, Indiana, have developed a parallel version of a Dupuit-Forchheimer flow model for regional modeling of 3-D flow in unconfined stratified aquifers.

2.4.7 Computing and Software Development Infrastructure

2.4.7.1 Software Quality Control

The quantity of software being developed and in use is increasing exponentially. Consequently, it is critical to establish protocols to ensure software integrity. A set of eleven Standard Operating Procedures (SOPs) was established to guide Quality Control and Quality Assurance. These were also incorporated into the National Exposure Research Laboratory Quality Assurance program (U.S. Environmental Protection Agency, 1995a). Seven of the SOPs are related to software quality control. These include:

- Quality assurance requirements in contracts and cooperative research agreements;
- Quality assurance of data sets and code in the Models-3 system;
- Computer security procedures;
- Disk and tape management procedures;
- Electronic transfer of emission inventory data;
- Transfer of spatial data; and
- Quality assurance of modeling framework and science code.

2.4.7.2 Software Configuration Management

Configuration management is a formal software engineering discipline that provides stability to the evolution of software products with the purpose of enhancing their integrity, quality, and reliability in a visible and traceable manner. A software configuration management plan was established in the Division to provide scientists, software developers, and users with the methods and tools to establish software baselines, control changes to those baselines, record and track their status, and audit their development. This approach applies to source code; executable load modules (object code); test data; database structures and element definitions; data libraries; control directives; job control language, procedures, rules, and associated documentation; and data pertaining to the development, operation, and maintenance of Models-3 and other production modeling codes such as RADM. The use of formal configuration management is an integral part of the quality assurance effort of the Division.

2.4.7.3 Files and Tapes Management

During the transition from a VAX to a Unix environment, the Division moved numerous files and tapes to Unix workstations using ftp. Tape backups were simplified by using VAX VMS backup, which can be converted using a system called Storage Management and moved to the IBM mainframe silo. The central archive management system can be used from any platform to restore data from tapes in the IBM silo. There were 16 disk packs and hundreds of tapes to be accessed. Each disk pack could hold over 2 million blocks of data. The clean-up was carried over to the IBM mainframe. The number of files on the IBM system was reduced from 82,000 to 60,000 and the number of tapes was reduced from 3,000 to 1,700.

2.4.7.4 Division World-Wide Web Home Page

The Division home page for the World-Wide Web was updated. This page includes an overview of the Division's mission; a staff directory with phone numbers and addresses; a map of the Research Triangle Park, North Carolina, area; a link to the Division Library’s home page; a list of Division publications; the FY-1995 annual report; monthly highlights; and links to sites that provide computer models and databases. The Division's Uniform Resource Locator (URL) address is http://www.epa.gov/asmdnerl/. The Internet anonymous ftp site (monsoon.rtpnc.epa.gov) includes databases and air quality simulation modeling programs developed or supported by the Division. Computer files are available for the following: acid deposition modeling, photochemical oxidant (smog) modeling, hazardous release modeling, particulate modeling, toxic modeling, emissions modeling (biogenic and anthropogenic), and associated meteorological models and data.

2.4.7.5 Division Intranet Development

A local Intranet was deployed to establish a full-function environment for information sharing, communication, and application. The Intranet was built on top of open networking technologies and standard Internet technologies. The Division’s Intranet now includes a number of key components to assist scientific software development, including a user guide for computer resources, links to division home pages, and links to in-house developed software tools. These include a request and authorization tool used for monitoring and requesting help for computer related problems and a tape archive tool for creating tape archive storage sets. These tools are made of HTML-based interface to an Oracle database, Common Gateway Interface (CGI), OraPERL scripts for accessing the database, and additional CGI scripts for housekeeping purposes.

2.4.8 Biogenic Emissions

The 1995 release of the second version of the Biogenic Emissions Inventory System (BEIS2) prompted a flurry of emission verifications and ozone modeling activities. The isoprene emissions estimated with BEIS2 increased by a factor of five over the earlier BEIS1 estimates. Confirmation for these higher BEIS2 isoprene emissions was suggested by Guenther *et al*. (1996) and Chang *et al*. (1996). Organizations such as the Ozone Transport Assessment Group and California Air Resources Board began to closely examine the role of biogenic volatile organic compounds (VOC) and nitric oxides (NO_x) in ozone modeling applications (Jackson *et al*., 1996). The Division was active in providing BEIS2 to the air pollution community, in integrating BEIS2 into regional air quality simulation models, and in developing BEIS3.

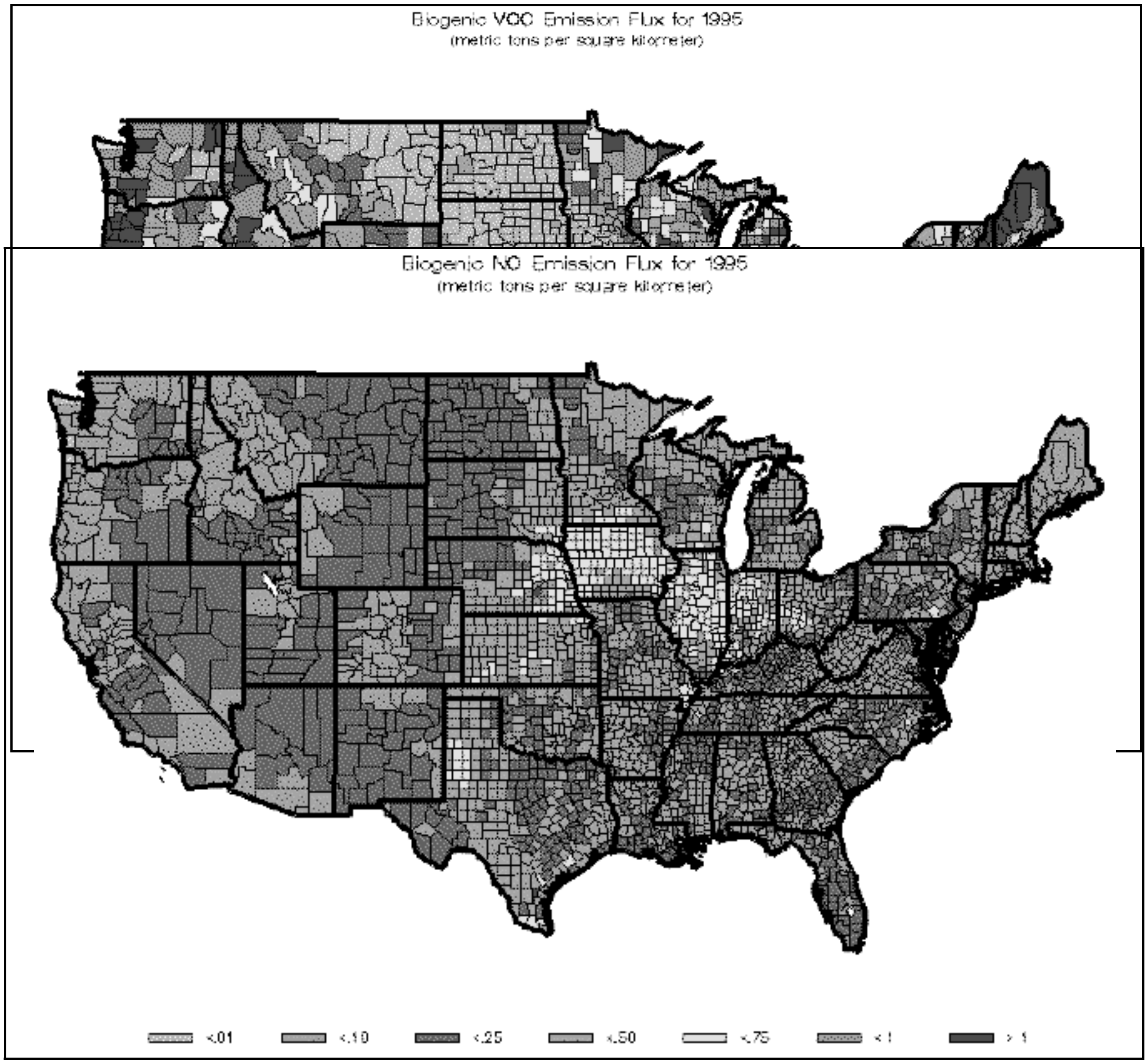
A Division scientist co-chairs a biogenic emissions committee sponsored by the State and Territorial Air Pollution Program Administrators/Association of Local Air Pollution Control Officials/EPA Emission Inventory Improvement Program (EIIP). The role of this committee is to develop a consistent and improved methodology for estimating biogenic emissions related to the CAA. A preferred methods document for estimating biogenic emissions was published by Adams (1996). It is available on the Division's Web site (www.epa.gov/asmdnerl/biogen.html) via anonymous ftp.

To satisfy a request from the EPA Office of Air Quality Planning and Standards (OAQPS), Pierce and Dudek (1996) used BEIS2 to estimate annual United States biogenic emissions for 1995. The highest VOC fluxes occurred in areas with a high percentage of forests, particularly those forests dominated by high-isoprene-emitting species such as oak, poplar, and spruce. The emissions pattern for VOC is shown in Figure 1. NO emissions are concentrated in areas with intensive agricultural activity, especially in the Midwest as shown in Figure 2.

Analysis continues on the isoprene flux experiment held in 1995 at the NOAA Atmospheric Turbulence and Diffusion Division’s (ATDD) Walker Branch site in 1995. This experiment, performed in concert with the Southern Oxidant Study's Nashville Ozone Field Experiment, involved researchers from NOAA ATDD, NCAR, Boulder, Colorado, Washington State University, Pullman, Washington, and the EPA National Risk Management Research Laboratory. Lamb *et al*. (1996) presented results that confirmed the isoprene emission factor for oak, the largest contributor to the isoprene emission inventory, and examined the role of canopy light and leaf temperature models.

Work is proceeding on in-house development of BEIS3. This new version will likely include VOC emission factors by forest species (instead of genus), 1-km or 4-km spatially resolved vegetative cover data (instead of county averages), and improved environmental correction algorithms. Adaptations of the Yienger and Levy (1995) soil NO_x emissions algorithm are also being considered.

The Division began to interact with the North Carolina Department of Environmental, Health, and Natural Resources (DEHNR) to examine nitrogen deposition to the eastern North Carolina watersheds. This subject is of concern because of eutrophication that has occurred during recent summers along the Neuse River and the rapid growth in swine production in the State, with total production estimated to be 9.5 million swine in 1998. A Division scientist worked with DEHNR to examine ammonia emission factors from swine management practices and to compare these emissions with other airborne nitrogen sources such as fossil-fueled power plants, mobile sources, agricultural soils, and lightning. A preliminary calculation indicated that nitrogen emissions from swine production may contribute 25 percent to the total nitrogen atmospheric inventory in North Carolina. Future efforts will involve nitrogen deposition modeling with RADM.



Biogenic VOC Emission Flux for 1995
(metric tons per square kilometer)
Biogenic NO Emission Flux for 1995
(metric tons per square kilometer)
<.01
<.10
<.25
<.50
<.75
< 1
> 1

Figure 1.

Figure 2.

For the second summer in a row, Washington County in eastern North Carolina was the site of a soil NO_x flux experiment. Several groups participated in this study including EPA, University of Maryland, College Park, Maryland, Air Resources Laboratory, Argonne National Laboratory, Argonne, Illinois, NASA Langley, Hampton, Virginia, and the host institution North Carolina State University, Raleigh, North Carolina. Preliminary results of the experiment were presented (Aneja and Gay, 1996). Preliminary results by Gao *et al*. (1996) indicate that chambers may provide an upper-estimate of the actual NO_x flux into the atmosphere above agricultural soils. During the upcoming year, the Division intends to continue work on verifying biogenic emission algorithms, on analyzing the sensitivity of biogenic emissions in ozone modeling applications, and on developing future biogenic emission algorithms.

2.4.9 Improvements in Land Use Data

A comprehensive land use data set was prepared for BEIS2. The data set relies on United States forest inventory statistics in the eastern United States, agricultural statistics, urbanized boundaries from the 1990 United States Census, and land use classifications from the Advanced Very High Resolution Radiometer (AVHRR) satellite. The AVHRR data were not used extensively because of the inability to accurately provide percentage of forest coverage in the eastern United States and to define urban areas. Efforts are being made in-house to more effectively couple the AVHRR data to spatially distribute and refine county-level statistics on agriculture, forest species coverage, and urbanized areas. It is anticipated that this new land use data set will be prepared for BEIS3 during 1997.

2.4.10 Working Group for Climate Services

The Working Group for Climate Services is part of the Interdepartmental Committee for Meteorological Services and Supporting Research sponsored by the Office of the Federal Coordinator for Meteorological Services and Supporting Research. This group met twice during FY-1996. A two-page internal document developed by this group defines climate services as:

> Climate services involve applying past weather information and results from models and other tools to provide decision-makers information on the weather and climate to expect in the future. The products of climate services are generally applied to timeframes beyond those addressed in conventional weather forecasts, but they may also be used by meteorologists to improve those forecasts.

The working group consists of representatives from ten federal agencies. The representatives give agency status reports including available data sets and data sets under development. One issue of concern is the continuity of observational systems. The working group also invites representatives of clients of climate services to attend and present their views on climate services.

2.4.11 US-Canadian Air Quality Agreement, 1996 Progress Report

The major part of Section III, *Progress: Scientific and Technical Activities and Economic Research* was compiled from inputs provided by the Subcommittee II of the Canada/United States Air Quality Committee. The reports state that wet sulfate deposition continues to decrease. Wet nitrate deposition and precipitation acidity showed no consistent change. Based on modeling, the prediction is that most of northeastern United States and lower Canada will experience a 30 percent reduction by 2010. Decreases in sulfur deposition were accompanied by decreases in sulfate concentrations of surface waters in that region. Limited improvements in water quality were found. Models also indicated that continued nitrogen deposition at current levels could erode benefits of sulfur emission controls. Lake monitoring in the Adirondacks showed a recent decrease in lake nitrate concentration (U.S. Environmental Protection Agency, 1996c).

2.5 Applied Modeling Research Branch

The Applied Modeling Research Branch investigates and develops applied numerical simulation models of sources, transport, fate, and mitigation of air toxic pollutants in the near field, and conducts research to develop and improve human exposure predictive models, focusing principally on urban environments where exposures are high. Databases are assembled and used for model development and research on flow characterization, dispersion modeling, and human exposure. Research is coordinated with other agencies and researchers.

2.5.1 QA/QC Guideline Development for Ground-Based Remote Sensors

The project addressed the development of quality assurance (QA) and quality control (QC) guidance for ground-based remote sensors (Doppler sodars, wind profiling Doppler radars, and radio acoustic sounding systems) for use in regulatory monitoring. This included revisions to the *Quality Assurance Handbook for Air Pollution Monitoring Systems, Volume IV: Meteorological Measurements* (U.S. Environmental Protection Agency, 1995b). The ground-based remote sensor characterization study was conducted in April 1995 at the Boulder Atmospheric Observatory in Boulder, Colorado. The results will be used for developing guidance on issues such as siting, installation, acceptance testing, calibration, auditing, routine operation and maintenance, tear-down, refurbishment, and expected accuracy as a function of atmospheric conditions and sensor configuration. A description of the experiment and goals of the QA/QC effort is outlined in Crescenti (1996). An overview of Doppler sodar intercomparison experiments is summarized by Crescenti (in press) with discussions on typical problems that are encountered with sensor performance.

2.5.2 Atmospheric Ozone Data Analysis

The EPA maintains monitoring sites to measure daily total column ozone and spectral ultraviolet (UV) radiation at seven locations in the United States. Atmospheric ozone mediates the surface flux of UV-B radiation. Long-term measurement of the total column ozone (stratospheric plus tropospheric) is necessary to determine seasonal and secular trends in ozone and corresponding surface radiation. Measurements are obtained using Brewer spectrophotometers. A comparison of total column ozone measurements obtained using the ground-based Brewer instruments was made with similar measurements obtained using the Solar Backscattered Ultraviolet Radiometer (SBUV/2) instrument aboard NOAA TIROS-N series satellites for the corresponding latitude and longitude. A comparative analysis of Brewer data obtained at six monitoring locations, with corresponding coincident and collocated SBUV/2 data, determined relative mean bias, correlation, comparability, precision, and completeness for each site. Correlation coefficients ranged from 0.67 at Riverside, California, to 0.87 at Boston, Massachusetts. Brewer measurements were generally higher than SBUV/2 measurements, with five of six sites recording positive mean bias ranging from +5.5 to +13.6 Dobson Units (2% to 5% relative mean bias). A seasonal model ($A + B \times \cos(2\pi(t-C))$) was used with Brewer and SBUV/2 data, and model mean, amplitude, and phase determined for each site. Model phase differences between Brewer and SBUV/2 (relative temporal offset) were significant for three of six locations, with SBUV/2 phase lagging Brewer phase by 0.03 year, or about 11 days, for Boston, Massachusetts, Bozeman, Montana, and Washington, DC. A delayed SBUV/2 response to perturbations in surface-ozone concentrations may explain some of the observed phase lags. A journal article is being prepared to show the results of this data analysis.

2.5.3 Agricultural Health Study

The Agricultural Health Study seeks to identify and quantify pesticide exposures to farmers, and indirect exposures to their families. A total exposure assessment methodology was incorporated into the design of the study, e.g., multi-media transport and multi-pathway exposure. Sampling design included air inhalation, oral ingestion, and dermal absorption. A draft report details the air transport and inhalation exposures monitored during the second phase, six-farm pilot study in Iowa and North Carolina. Meteorological data were collected from an on-site three-meter tower. Outdoor air was sampled on the day of the pesticide application event, and indoor air samples were collected on three consecutive days centered on the application day. Personal activity logs, indicating time and location, were maintained by participants during the monitoring period. Of 33 targeted pesticides, 7 were applied on at least one of the participant farms, 11 were detected in the outdoor air near a farm residence, and 17 were detected in the indoor air of a farm residence. Indoor concentrations of the applied pesticides were detected on four of the six farms, however, there is no conclusive evidence to support an outdoor air source of indoor concentrations of applied pesticides. Indoor concentrations of non-applied pesticides were more the rule than the exception. On five of the six pilot-study farms, concentrations of non-applied pesticides were detected in the indoor air samples on at least one day. As expected, the applicator's inhalation exposure to applied pesticides is greater than that of any other family member on the day of application. For spouse and children, the indoor microenvironment contributed to inhalation exposure of pesticides to a far greater extent than did the outdoor-on-farm microenvironment; even on the day of pesticide application.

2.5.4 Lake Michigan Mass Balance Project

The Lake Michigan Mass Balance (LMMB) project utilizes a mass balance approach to develop a lake-wide management plan to address toxic pollutants in Lake Michigan. The primary goal of the mass balance study is to develop a sound, scientific base of information to guide future toxic load reduction efforts at the state and Federal levels for Lake Michigan. The principle objectives of the modeling portion of this effort are to estimate the atmospheric deposition and air-water exchange of priority toxic pollutants. This includes the description of the spatial and temporal variability over Lake Michigan; evaluation of the magnitude and variability of toxic chemical fluxes within and between lake compartments, especially between the sediment and water column and the water column and the atmosphere; development of contaminant concentration forecasts in water and sediment throughout Lake Michigan, based upon meteorological forcing functions and future loadings using load reduction alternatives; and quantification of the uncertainty in estimates of tributary and atmospheric loads of priority toxic pollutants and model predictions of contaminant concentrations.

During FY-1996, a multi-year plan was developed and designed to use ongoing modeling systems research and expertise of the Division personnel. Division scientists became familiar with the hydrodynamic and water quality modeling components to be used in the linked system. Possible points of water column and atmospheric model interaction were identified. The Division will model the atmospheric fate and transport of atrazine. It was determined that a sampled atrazine emission inventory of sufficient temporal and spatial detail was not available, and an appropriate, partially validated emission model was identified. A modified version of MM5 will interface with the emission model and will act as the principal emission model driver. Both meteorological and emission databases will be completed during FY-1997.

2.5.5 Development of a Multi-Media Modeling Component for Endocrine Disruptor Exposure Research

Potential endocrine disrupting chemicals (EDCs) were identified as a new, relatively poorly understood source of environmental risk to biological health. An environmental endocrine disruptor was defined as an exogenous agent that interferes with the production, release, transport, metabolism, binding, action or elimination of natural hormones in the body responsible for the maintenance of homeostasis and regulation of developmental processes. In addition to the so-called environmental estrogens and anti-androgens, the term includes agents that affect the thyroid and pituitary glands and other components of the endocrine system. Potential EDCs include many used and banned agricultural chemicals such as DDT/DDE, aldrin, dieldrin, and atrazine, many PAHs (polycyclic aromatic hydrocarbons), PCBs (PolyChlorinated Biphynals), and such trace metals as mercury, lead, and arsenic.

In FY-1996, Division scientists lead an EDC exposure modeling team. The principal goal of the initial research is to identify the most critical science and knowledge gaps in the regional EDC transport system. A model objective plan was developed, which includes the acquisition of a relatively sophisticated hybrid compartmental model, qualitative model validation, and formal sensitivity analysis. Although regional, meso-scale, and local models will eventually be developed, only regional scale models will be employed in the near-term to determine principal inter-media pathways and media endpoints for selected candidate EDCs. Once the full regional modeling system is in place, Division scientists will focus on the atmospheric media compartment and inter-media transfer functions between the atmospheric compartment and water, soil, sediment, and vegetation compartments.

2.5.6 Statistical Modules and Advanced Mathematical Analysis Tools Developed for an Innovative Multi-Pollutant Exposure Model

The project addressed the Agency's need for improved methodologies for estimating the population exposures for use in its risk assessments. Using field sampling and data analysis, the project sought to address the need directly by developing a new exposure assessment methodology with a solid statistical framework. The goal is to develop a multi-pollutant exposure model, which will combine the latest research on human time/activity patterns; concentration levels for numerous locations both indoors and outdoors; air exchange rates for calculating indoor intrusion of ambient pollutants; spatial mapping of ambient pollution concentrations; meteorological effects on the distribution of pollutants; and emissions from specific sources with the calculation of exposure scenarios using rigorous mathematical and statistical techniques. A year of five-minute measurements were made of indoor and outdoor concentrations for carbon monoxide, ozone, and $PM_{2.5}$ (including PAHs bound to the $PM_{2.5}$) at the residential exposure project (REP) site. Data on CO, ozone, and PM_{10} and $PM_{2.5}$ were compiled from numerous ambient monitoring sites located throughout the San Francisco Bay area. Additionally, meteorological data from the area observation stations were compiled for the study period, which ran for 15 months.

The data on CO, ozone, and PM_{10} and $PM_{2.5}$ will be analyzed and used in the Total Human Exposure Model being developed. More detailed analyses of meteorological effects on the distribution and magnitude of the ambient pollutants will be made for the area as a whole, and on a finer spatial scale in the immediate vicinity of the REP site.

2.5.7 Modeling Pesticide Applications

In FY-1996, Division scientists continued their involvement in a program to develop methodologies for evaluating the drift of airborne pesticides from agricultural applications. This work is being performed through a cooperative research and development agreement (CRADA) with the agricultural chemical industry's Spray Drift Task Force (SDTF) and through a cooperative agreement between EPA and New Mexico State University, Las Cruces, New Mexico. The goals are to expand our understanding of the important mechanisms that affect off-target drift, by conducting major field studies, and to develop improved models of the transport, dispersion, and deposition of pesticides.

The CRADA with SDTF continues to be beneficial. Three major field studies of aerially applied spray drift have greatly enhanced the body of knowledge in the literature concerning off-target impacts. A review of these data and an overview of the parameters that are important to spray drift are found in Bird *et al.* (in press). A three-tiered approach for primarily modeling aerial pesticide applications is very near completion. The approach, referred to as AGDRIFT, is designed for estimating off-target deposition of aerially applied pesticides and for determining the buffer zones needed around sensitive aquatic and terrestrial habitats to protect them from undesired exposures. Tier one is a preliminary screen designed to yield exposure estimates typical of those encountered in the top 10 percent of application scenarios. Tiers two and three allow the user to increase the level of detail concerning the application parameters and the environmental conditions to obtain a more refined estimate of likely spray drift impacts in specifically controlled applications. Thus, this modeling approach should be a useful tool for users to determine the best and most cost effective practices for spray drift control. Additionally, the EPA Office of Pesticide Programs will use this model to evaluate the potential environmental impacts of new pesticide formulations.

AGDRIFT is being evaluated by comparing its results with the data from the three SDTF field studies of aerial drift. The databases were evaluated and found to be of high quality with a useful range of application and environmental conditions (Bird and Perry, 1996). Preliminary results of the model comparisons against the field data show that AGDRIFT is performing very well immediately downwind of the treated field. However, beyond about 300 meters downwind, the model shows a tendency to overpredict the measured deposition by typically 50 percent or more. This downwind bias is believed to be partly due to problems in the data related to tracer loss from the deposition plates and to the model's simplistic handling of evaporation. Both problems are being further investigated.

The cooperative agreement with New Mexico State University is focused on the drift of pesticides from orchard canopies treated with pesticides using air-blast application techniques. These special cases involve the use of very high-speed fans literally blasting the aspirated pesticides up through the foliage. In an effort to reach the entire canopy, overspray becomes available for off-target drift. There are issues related to turbulent transport and dispersion through and beyond the canopy, resulting in unwanted drift. Through this cooperative agreement, a drift model related to air-blast spraying is being developed.

The orchard model is numerically based with major components, that include a two-dimensional simulation of micrometeorological variables in and around the canopy, a Lagrangian in-canopy droplet transport and deposition module, and a characterization of air-blast sprayer emissions. Initially, the model will provide steady-state estimates of droplet deposition staying within the canopy and estimates of spray material passing beyond the canopy boundaries, vertically and horizontally. A field study conducted in a mature pecan orchard located in southern New Mexico is providing a basis for further understanding of orchard spray drift and for evaluation of the model. Data collected during the field study in the summer of 1996 include information on the drop size, number, and velocity distribution of droplets released from the sprayer zone; vertical distribution of tree, stem/foliage area, density, size and orientation of the plant canopy elements; and vertical profiles of the wind field, turbulence, temperature, humidity, and radiation within and above the canopy. Malathion was used as a tracer for assessment of flux and deposition at sites placed horizontally from about 5 tree heights upwind to about 23 tree heights downwind of the spray line and vertically from the surface to about 3 tree heights. The spray cloud was sampled with conventional collectors (string collectors, hi-vol samplers, filter paper, etc) and with remote sensing using a LIDAR and thermal scanner. Analysis of the field data is underway.

2.5.8 Wind Tunnel Experiments on Dense Gas Diffusion

Using three wind tunnels, a collaborative effort focusing on improving algorithms for vertical diffusion of dense (heavier-than-air) gases has given added value to field studies of dense gas behavior. Authorized by the 1990 CAAA, dense gas studies began in 1993 under the Chemical Hazards Atmospheric Releases Research (CHARR) program. Division personnel conducted dense gas studies in the FMF wind tunnel in collaboration with the Petroleum Industry Research Forum (PERF), which had sponsored a major field experiment in FY-1995 at the Spills Test Facility, Nevada Test Site, Las Vegas, Nevada. Division personnel provided support to PERF in planning and monitoring dense gas studies in a wind tunnel at the University of Surry, Guildford, England, which is uniquely capable of producing stable boundary layers. Finally, with the support of the Department of Energy, the Chemical Hazards Research Center at the University of Arkansas, Fayetteville, Arkansas, cooperated closely with the Division to carry out parallel studies in its especially designed wind tunnel.

All three wind-tunnel studies focused on vertical entrainment, mixing with ambient air at the top of the dense gas plume, over rough surfaces that better simulated land surfaces than smooth floors used in past dense gas wind tunnel studies. The FMF experiments used exactly the same roughness geometry used for the uniform roughness array portion of the August 1995 field experiments (Poole-Kober and Viebrock, 1996). These studies were aimed at providing the best comparison possible between results of field and wind tunnel experiments, and for defining future wind tunnel work at the lowest possible Reynolds number (Re) for acceptable simulations. Re is proportional to element height times wind speed, and very low-wind speeds are required to simulate full-scale dense gas behavior. To facilitate Re studies and to extend the range of distance and elements height studied, two series of experiments were done; one with 2" high roughness and the other with roughness only 1/6 as high. The latter gave good simulations only when the wind speed was raised to 1 m/s or higher. This firmly established the minimum Re criterion needed to improve the design of the experiments in England.

Experiments at all three locations used, or will use, a wide range of dense gas (CO_2) flow rates to vary the plume Richardson number (Ri), a measure of the degree of suppression of turbulence and vertical entrainment by the heaviness of the gas. The two FMF series at different scales gave almost identical (normalized) entrainment rates for the same Ri, as long as the minimum Re was maintained. A series as identical as possible to the large-roughness FMF series was run in the Arkansas wind tunnel. The preliminary results show agreement on entrainment rate vs. Ri in the 10% to 20% range. A second series was run in Arkansas over a different roughness array chosen for contrast; yet, the preliminary results look similar. The University of Surrey developed new instrumentation for measurement of turbulent fluxes at very small scales and developed a system for producing a strongly stable boundary layer, as required by PERF.

2.5.9 CAPITA Monte Carlo Model

The CAPITA (Center for Air Pollution and Trend Analyses) Monte Carlo Model was developed by Husar and Patterson (1981). During FY-1996, efforts continued to implement the original Monte Carlo Model onto the IBM-PC platform. A Beta version of the model was tested, and plans were made to distribute a final version over the Internet in FY-1997. The new Monte Carlo model was designed in a modular framework, separating the emissions, transport, and kinetics calculations. The transport module employs a Monte Carlo technique for the simulation of atmospheric boundary layer physics. The Monte Carlo model employs multiple-layer mixing in the calculation of the back trajectories, using a random process such that no two trajectories calculated for the a given receptor and receptor time are the same. This allows for each receptor air mass to be simulated by multiple trajectories. Different techniques are being examined for integrating the wind fields when calculating the trajectories. Kinetic chemical processes are simulated using first order rate equations where the kinetic rate coefficients vary in space and time. The rate coefficients are determined via a tuning process comparing simulated and actual measurements.

A Web based server for the model is being developed to allow for the calculation of North American trajectories from 1991 through 1995 interactively over the Internet. The main design paradigm of the software is the client-server architecture. The client is the part of the software that interfaces the user with the Monte Carlo Model. It has two components: the query input, which specifies the process to be computed, e.g., creation of air mass histories, simulated concentration fields, etc.; and the data output and visualization that presents the resulting data files to the user. The client software uses multiple windows and forms to specify the query. The output from the trajectory server would be a multi-dimensional array (hyperslab). The client-server architecture follows the concepts and developments in modern relational database management systems. The server itself consists of a query processor and the Monte Carlo model processors. The query processors translate the input query into specific actions to be executed. The Monte Carlo Model then performs the queried actions, such as calculating trajectories by integrating the equation of motion using Eulerian wind fields.

The output is a multi-dimensional array, which can then be displayed by rendering the program in the client software. The Eulerian/Lagrangian transformer allows for the creation of air mass histories for individual locations at any 3-D point in the modeling domain. The air mass histories can be created from either a source or receptor view point, thereby identifying the transit of pollutants from a source or an air mass to a receptor. The resulting data sets can then be used to characterize air flow and provide meteorological information of air masses to the receptor. Such data is valuable in the interpretation and analysis of air quality data. A map view was developed to identify the air mass pathway, while a time history view was developed to show the variation in trajectory height, relative humidity, temperature, and precipitation.

2.6 Air Policy Support Branch

The Air Policy Support Branch supports activities of the EPA Office of Air Quality Planning and Standards (OAQPS). The Branch responsibilities include: (1) evaluating, modifying, and improving atmospheric dispersion and related models to ensure adequacy, appropriateness, and consistency with established scientific principles and Agency policy; (2) preparing guidance on applying and evaluating models and simulation techniques that are used to assess, develop, or revise national, regional, state, and local air pollution control strategies for attainment and maintenance of National Ambient Air Quality Standards (NAAQS); and (3) providing meteorological assistance and consultation to support the OAQPS in developing and enforcing Federal regulations and standards and assisting the EPA Regional Offices.

2.6.1 Modeling Studies

2.6.1.1 Evaluation Methodologies

An invited paper was presented on model evaluation methods (Irwin and Lee, 1996) at the 4th Harmonisation Workshop held in Oostende, Belgium, May 6-9, 1996. Results were summarized of ongoing investigations aimed toward updating and refining methods available for evaluating performance in relatively simple terrain of point source dispersion models. Analyses of near-surface and buoyant-elevated tracer releases suggest that natural variability is sufficiently large that model evaluation methods are best designed to provide an ensemble of observations for comparison with modeling results. When models only simulate the ensemble average concentration values for each specified boundary condition, comparisons with observations are best restricted to comparisons of observed and estimated median normalized concentration values for each ensemble. Unbiased models would be expected to compare favorably with the median observed concentration values. In principle, all other factors being equal such models would be expected to underestimate the observed maxima within an ensemble, and overestimate the observed minima within an ensemble. The ongoing collaboration with international scientists is an effort to develop consensus on how to assess and define model performance and develop standards.

2.6.1.2 Urban Air Toxics Study

The Clean Air Act requires the regulation of hazardous air pollutants in urban areas. In a study conducted in four U.S. cities, an integrated exposure and risk assessment approach uses a comparison of emissions and relative health risk attributed to emissions from major stationary, area, and mobile sources of five key pollutants. Using emission inventories, the Industrial Source Complex (ISC3) dispersion model will be applied to various emission reduction scenarios targeted at the various sources to assess impacts and costs. This Gaussian plume model has a long history in assessing pollutants from a wide variety of point, area, and mobile sources. In this application, seasonal average hourly concentrations are needed to determine annual cancer risk incidences. The use of a photochemical grid model such as UAM was considered. However, UAM does not treat four of the five pollutants in the study; does not provide adequate winter season estimates; cannot account for the effects of particulate deposition; is episodic; and thus, does not run for an entire year. Considerable effort is required in designing the modeling study since there is a court-ordered mandate.

2.6.1.3 AMS/EPA Regulatory Model Improvement Committee

In 1991, the AMS and EPA joined in a collaborative effort to introduce advances in boundary layer meteorology into regulatory dispersion models. During FY-1996, work concentrated on improving characterization of the stable boundary layer; improving characterization of near-ground level dispersion; and developing a more elegant urban boundary layer formulation. The results of the work in the early part of the fiscal year are documented in Cimorelli *et al*. (1996).

Also, the committee addressed areas highlighted by internal peer reviewers. Based on internal peer reviewers' comments, the parameterization of turbulence with height was revised so that values at the top of the boundary layer are independent of surface conditions (Cimorelli *et al*., 1996). Additional work is underway to resolve problems identified through the developmental evaluation. Separate expressions are used for turbulent dispersion from ground-level sources than from elevated sources. Work is proceeding on an appropriate expression for the transition between formulations for ground-level sources and elevated sources.

A continuing developmental evaluation of the model allows various components to be tested, corrected, and, if necessary, replaced with alternative algorithms. For example, the treatment of the urban boundary layer changed because of the developmental evaluation. It is known that urban turbulence differs from rural turbulence due to the difference in surface roughness and change in heat flux. Heat flux changes are due to space heating and heat absorbed and re-emitted by the concrete and asphalt structures in the urban area.

The reviewers questioned whether the urban anthropogenic component of the heat flux needed to be accounted for in the model to produce reasonable results. The Indianapolis data (Murray and Bowne, 1988) (nighttime only) was run with and without the addition of an anthropogenic urban-heat flux term of 50 watts per square meter, an amount found appropriate for Indianapolis by Hanna and Chang (1991). The results (unpaired) are shown as quantile-quantile (Q-Q) plots in Figure 1. The Q-Q plot in Figure 1a shows a strong tendency for AERMOD (AMS/EPA Regulatory model) to over predict high quantile concentrations above the 97th percentile and to under predict low quantile concentrations when anthropogenic heat flux is not included. The plot goes off scale at about the 84th percentile point. When anthropogenic heat flux is included, modeled values compare much more closely to the observed, with modeled and observed ratios ranging between 0.7 and 1.7, at all quantile levels represented in Figure 1b. This plot intersects the border of the chart at about the 16th percentile point. Based on these results, the decision was made to include anthropogenic heat flux in AERMOD. An algorithm for the model is being developed that scales the anthropogenic heat flux to the size of the city.

2.6.1.4 Regional Modeling for Regulatory Applications

In support of the EPA review of the ozone National Ambient Air Quality Standards (NAAQS), ROM was used in FY-1996 to examine the cost-benefit of potential new NAAQS. Emission reduction targets based on local controls were compared to region-wide emission reduction targets across the eastern United States. While benefits are achieved by some regional reductions, significant local emission controls will be needed in most ozone problem areas. The ROM predictions from these simulations were used to derive least cost, source-specific control strategies that match the emission reduction targets. These

a. b.

Figure 5. Quantile-Quantile plots of modeled versus observed concentrations, for Indianapolis data, with and without inclusion of anthropogenic heat flux in the modeling.

specific strategies will be simulated in FY-1997 to quantify the benefits of improvements in air quality relative to the proposed NAAQS.

Attainment of the ozone NAAQS is complicated by the influence of regional pollution transport on large areas of the eastern United States. In recognition of this problem and in conjunction with the Environmental Council of States (ECOS), the EPA established the Ozone Transport Assessment Group (OTAG). The mission of OTAG is to recommend to EPA specific regional emission controls. When implemented, these controls will reduce the transport component of the ozone problem, enabling States to attain the ozone NAAQS through various additional local control programs.

The assessment of the relative benefits of potential strategies by OTAG is based on photochemical modeling using UAM-V. Compared to ROM, UAM-V has enhanced features including plume-in-grid treatment, multiple-nested grids, and increased vertical resolution. Over 20 emission scenarios were simulated for each of four ozone episodes ranging in duration from 9 to 15 days each. Examples of the type of results from these simulations are shown in Figures 6 and 7. The model predictions of daily peak ozone across the eastern United States for a key day in the July 1988 episode are shown in Figure 6. The emissions in this scenario reflect the net effects of predicted economic conditions and control programs required by the CAA to be implemented by the year 2007. Although ozone may decline over the next 10 years as a result of the mandated programs, there may still be a regional problem that will require additional controls. The estimated impact of a possible regional control strategy, involving reductions in automotive as well as industrial emissions, is predicted to result in widespread decreases in ozone, as shown in Figure 7. The largest ozone reductions are located near and downwind of urban areas and clusters of rural industrial sources (i.e., the Ohio Valley). Localized increases in ozone are associated with reduced emissions of nitric oxide in areas where these emissions actually reduce ozone.

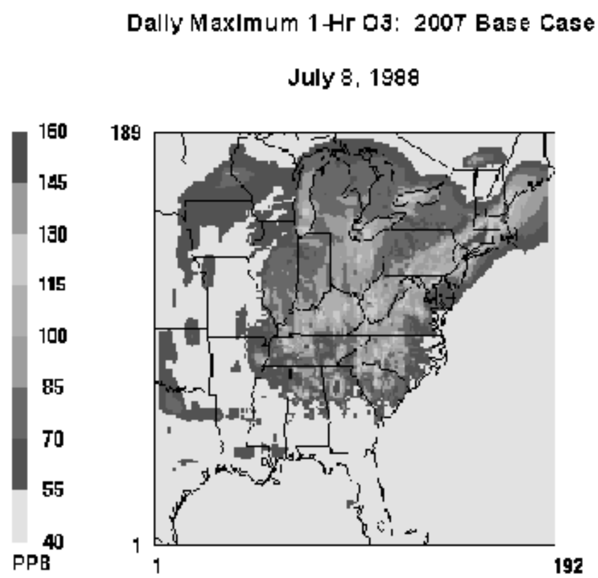


Figure 6. Daily maximum one-hour ozone concentration predictions for the July 8, 1988, ozone episode using the 2007 base case reduction scenario.

2.6.2 Modeling Guidance

2.6.2.1 Support Center for Regulatory Air Models

During FY-1996, several activities were accomplished. The SCRAM (Support Center for Regulatory Air Models) BBS (Bulletin Board System) was made accessible via Internet using two different servers. First, all SCRAM files were transferred to the EPA server, Earth1. The URL address for this site is http://www.epa.gov/scram001. Second, SCRAM and TTN were made available via the TTN2000 Web site, which contains other technical information areas. The SCRAM Web site has the same appearance and advantages as the SCRAM BBS. In addition, *CALPUFF Conferencing* was created to facilitate using and testing of the CALPUFF modeling system.

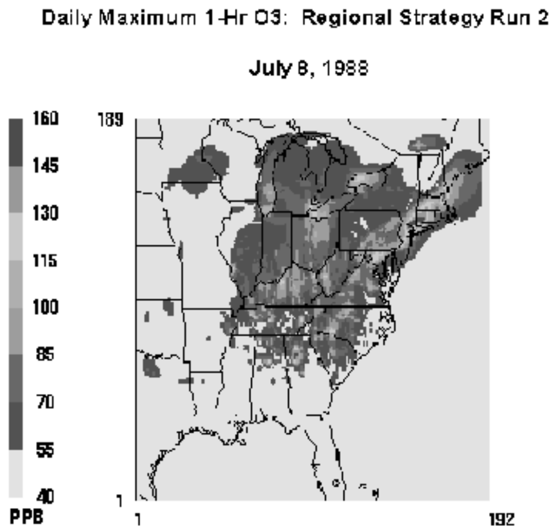


Figure 7. Same as figure 6 using the regional strategy incorporating both automotive and industrial emission reductions.

2.6.2.2 Expert Interface to the Industrial Source Complex Model

ExInter is a Windows-based interface system added to the EPA ISC3 model. ExInter enables non-expert air modeling personnel to build input files and run the ISC3 model and its preprocessor for routine applications. ExInter was developed to help Superfund personnel and regional offices perform routine air dispersion modeling analyses of emissions from hazardous waste disposal sites. The system has gained acceptance by State and local air pollution control agencies because it facilitates training and increases resource efficiency. ExInter encourages users to be thorough and, early in the process, to consider data needs and relevant issues regarding the modeling applications; thereby, encouraging consistent and uniform modeling practices. The model was placed on the EPA Electronic Bulletin Board for public distribution.

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APPENDIX A: ACRONYMS, ABBREVIATIONS, AND DEFINITIONS

ACM	Asymmetric Convective Model
ADOM	Acid Deposition and Oxidant Model
AERMIC	AMS/EPA Regulatory Model Improvement Committee
AERMOD	Improved ISCST2 Model
AGDRIFT	AGricultural spray DRIFT model
AMS	American Meteorological Society
AQM	Air Quality Model
ASD	Accurate Spatial Derivative
ASMD	Atmospheric Sciences Modeling Division
ATDD	Atmospheric Turbulence and Diffusion Division (NOAA)
AVHRR	Advanced Very High Resolution Radiometer
BASC	Board on Atmospheric Sciences and Climate (NAS/NRC)
BEIS	Biogenic Emissions Inventory System
CAA	Clean Air Act of 1970
CAAA	Clean Air Act Amendments of 1990
CALPUFF	CALifornia PUFF model
CAMRAQ	Consortium for Advanced Modeling of Regional Air Quality
CASTNET	Clean Air Status and Trends NETwork
CB4	Carbon Bond 4
CBL	Convective Boundary Layer
CCIC	Committee on Computing, Information, and Communication (NSTP)
CD-ROM	Compact Disk – Read Only Memory
CENR	Committee on Environment and Natural Resources
CHARR	Chemical Hazards of Atmospheric Releases Research
CRADA	Cooperative Research And Development Agreement
CREME	Cooperative REgional Model Evaluation project
CTM	Chemistry Transport Model
DEHNR	Department of Environment, Health and Natural Resources (North Carolina)
DOE	Department of Energy
ECOS	Environmental Council of State
EDC	Endocrine Disrupting Chemicals
EDSS	Environmental Decision Support System
EIIP	Emission Inventory Improvement System
EMEP	European Monitoring and Evaluation Program
EPA	Environmental Protection Agency
EUROTRAC	EUROpean experiment on the TRAnsport and transformation of trace atmospheric Constituents
ExInter	Expert Interface
F*	non-dimensional bouyancy
FACA	Federal Advisory Committee Act
FCMSSR	Federal Committee for Meteorological Services and Supporting Research
FDDA	Four Dimensional Data Assimilation
FMF	Fluid Modeling Facility (EPA)
FY	Fiscal Year
GEMAP	Geocoded Emission Modeling and Projection
GIS	Geographical Information System
GOES	Geostationary Operational Environmental Satellite
HPCC	High Performance Computing and Communications program
HTML	HyperText Markup Language
IBM	International Business Machines
ICMSSR	Interdepartmental Committee for Meteorological Services and Supporting Research
IMPROVE	Interagency Monitoring of PROtected Visual Environments
I/O	Input/Output
IOV	Initial Operating Version
ISC3	Industrial Source Complex model – version 3
ITM	International Technical Meeting

IWAQM	Interagency Work Group on Air Quality Models
LISA	Labortoire Interuniversitaire des Systemes Atmospheriques
LMMBP	Lake Michigan Mass Balance Project
LMOS	Lake Michigan Ozone Study
LRPM	Lagrangian Reactive Plume Model
MEPPS	Models-3 Emission Processing and Projection System
MESOPUFF	MESOscale Lagrangian PUFF dispersion model
MFL	Mobile Flux Laboratory
MIDPRO	Models-3 Input Data PROcessor
MLM	Multi-Layer inferential dry deposition Model
MM4/5	Mesoscale Meteorological Model — version 4/version 5
Models-3	Third generation air quality modeling system
MPP	Massive Parallel Processors
MPRM	Meteorological Processor for Regulatory Models
MSC-W	Modeling Synthesizer Center - West
NAAQS	National Ambient Air Quality Standards
NADP	National Acid Deposition Program
NAPAP	National Acid Precipitation Assessment Program
NARSTO	North American Research Strategy for Tropospheric Ozone
NARSTO-NE	NARSTO-NorthEast
NAS	National Academy of Sciences
NASA	National Aeronautics and Space Administration
NATO/CCMS	North Atlantic Treaty Organization Committee on Challenges of Modern Society
NCAR	National Center for Atmospheric Research
NDDN	National Dry Deposition Network
NERL	National Exposure Research Laboratory (EPA)
NESC	National Environmental Supercomputing Center (EPA)
NESCAUM	NorthEast States for Coordinated Air Use Management
NetCDFI/OAPI	Models-3 format
NMC	National Meteorological Center
NOAA	National Oceanic and Atmospheric Administration
NOVA	Natural emissions of Oxidant precursors: VAlidation of technique
NRC	National Research Council
NSF	National Science Foundation
NWS	National Weather Service
OAQPS	Office of Air Quality Planning and Standards (EPA)
ORD	Office of Research and Development (EPA)
OSTP/NSTC	Office of Science and Technology Policy/National Science and Technology Council
OTAG	Ozone Transport Assessment Group
PAH	Polycyclic Aeromatic Hydrocarbons
PAMS	Photochemical Assessment Monitoring Stations
PBL	Planetary Boundary Layer
PCB	PolyChlorinated Biphynals
PCP	Progran Control Processor
PDM	Plume Dynamics Model
PE	Program Element
PERF	Petroleum industry Environmental Research Forum
PM	Particulate Matter
Q-Q	Quantile-Quantile plot
QA	Quality Assurance
QC	Quality Control
RADM	Regional Acid Deposition Model
RASS	Radio Acoustic Sounding System
Re	Reynolds number
RELMAP	REgional Lagrangian Model for Air Pollution
REP	Residential Exposure Project
Ri	Richardson number
ROM	Regional Oxidant Model
RPM	Regional Particulate Model

SAEWG	Standing Air Emission Work Group
SARMAP	SJVAQS/AUSPEX Regional Modeling Adaptation Project
SASWG	Standing Air Simulation Work Group
SBUV	Solar Backscattered UltraViolet radiometer
SCRAM BBS	Support Center for Regulatory Air quality Models Bulletin Board System
SDTF	Spray Drift Task Force
SERDP	Strategic Environmental Research and Development Program
SOP	Standard Operating Procedure
SOS	Southern Oxidant Study
SVOC	Semi-Volatile Organic Compounds
TEQ	Toxic EQuivalent
TKE	Turbulent Kinetic Energy
TOMS	Total Ozone Mapping Spectrometer
TTM	Transilient Turbulence Method
UAM	Urban Airshed Model
UAM-V	Urban Airshed Model – Variable grid
URL	Uniform Resource Locator
USWRP	U.S. Weather Research Program
UV	Ultraviolet
VOC	Volatile Organic Compounds
WELSONS	Wind Erosion and Loss of SOil Nutrients in semi-arid Spain
WWW	World-Wide Web

APPENDIX B: PUBLICATIONS

Alapaty, K., R. Mathur, and D.W. Byun. A modeling study of vertical diffusion of passive and reactive tracers using local- and nonlocal-closure boundary layer schemes. In *Air Pollution and Modeling and Its Application XI*. Volume 21. S.-E. Gryning and F.A. Schiermeier (Eds.). Plenum Press, New York, NY, 433-442 (1996).

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APPENDIX C: PRESENTATIONS

Atkinson, D.G. Air pollution dispersion models — Applications. Presentation via video of updates to the Air Pollution Training Institute (APTI) Course 423 for the State of Georgia, Research Triangle Park, NC, November 11, 1995.

Atkinson, D.G. Air pollution dispersion models — Applications. Presentation via video of updates to the Air Pollution Training Institute (APTI) Course 423 for the State of Georgia, Research Triangle Park, NC, November 18, 1995.

Benjey, W.G. Demonstraton of Models-3 emission system. Televised workshop, North Carolina State University, Raleigh, NC, April 23, 1996.

Benjey, W.G. Status of the Models-3 emission processor. Presentation at the Third Models-3 Science Design Workshop, Research Triangle Park, NC, September 18, 1996.

Benjey, W.G. EIIP data model panel discussion. Presentation at Air & Waste Management Association Emission Inventory Conference, New Orleans, September 3, 1996.

Binkowski, F.S. Regional scale particulate matter: Preliminary analyses of current and future loadings in the eastern United States using a regional scale state-of-science model of airborne fine particles. Presentation at the 5th International Atmospheric Sciences and Applications to Air Quality Conference, University of Washington, Seattle, June 19, 1996.

Bullock, O.R., Jr. Air toxics modeling capabilities at EPA/NERL and plans for a multi-media modeling assessment of atrazine for the Lake Michigan Mass Balance Study. Presentation at the Lake Michigan Mass Balance Study, All Hands Meeting, Great Lakes National Program Office, Chicago, IL, December 6, 1995.

Bullock, O.R., Jr. Lagrangian modeling of atmospheric mercury for EPA's Mercury Study Report to Congress and possible applications to south Florida. Presentation at the South Florida Mercury Research Coordination Workshop, Orlando, FL, April 23, 1996.

Bullock, O.R., Jr. RELMAP atmospheric mercury modeling strategy and results for the NESCAUM mass-balance assessment. Presentation at the NorthEast States for Coordinated Air Use Management (NESCAUM) Mercury Workshop, Kennebunkport, ME, July 8, 1996.

Bullock, O.R., Jr. RELMAP atmospheric dioxin modeling strategy and preliminary results. Presentation at the EPA Dioxin Workshop on Deposition and Reservoir Sources, Washington, DC, July 23, 1996.

Bullock, O.R., Jr. Lagrangian modeling of mercury air emission, transport and deposition with source-type discrimination. Presentation at the 4th International Conference on Mercury as a Global Pollutant, Hamburg, Germany, August 5, 1996.

Burton, R.M., and J.J. Streicher. Influence of weather on aerosol exposure in selected, highly populated metropolitan areas of the United States. Presentation at the Measurement of Toxic and Related Air Pollutants Symposium, Research Triangle Park, NC, May 8, 1996.

Ching, J.K.S. Modeling PM for eastern United States. Presentation at the New York State Department of Health, Albany, NY, January 18, 1996.

Cooter, E.J. Introduction and overview of the short course “Climate Data and Information for Environmental Applications.” Presentation at the American Meteorological Society, Atlanta, GA, January 27, 1996.

Cooter, E.J. Expanding your Hhorizons: Careers in meteorology. Presented to seventh graders at North Carolina State University, Raleigh, NC, March 13, 1996.

Crescenti, G.H. Meteorological ground-based sensing. Presentation at the Regional Office/State/Local Agency Modeler’s Workshop, Research Triangle Park, NC, April 24, 1996.

Dennis, R.L. RADM results on the effectiveness of possible emissions reductions towards reducing deposition to the Bay watershed. Presentation to the Chesapeake Bay Shared Resources Conference/Workshop, Warrenton, VA, October 10, 1995.

Dennis, R.L. Analysis of photochemical dynamics affecting model state-variable predictions in the Regional Acid Deposition Model. Presentation at the American Geophysical Union meeting, Baltimore, MD, May 25, 1996.

Eder, B.K. Statistical Data Analysis. Presentation at the short course “Climate Data and Information for Environmental Applications,” at the American Meteorological Society, Atlanta, GA, January 27, 1996.

Eder, B.K. A rotated principal component analysis of total column ozone obtained from TOMS for 1984-1989. Presentation at the 2nd Annual North Carolina Environmental Science Research Fair, National Institute of Environmental Health Sciences, Research Triangle Park, NC, March 29, 1996.

Gillette, D.A. Get the real dirt about the atmosphere. Presentation at the local American Meteorological Society meeting, Research Triangle Park, NC, October 30, 1995.

Gillette, D.A. Modeling of the effect of vegetation on wind erosion. Seminar presented at Duke University, Durham, NC, October 30, 1995.

Gillette, D.A. Wind erosion modeling: Recent Jornada LTER results. Seminar presented at Duke University, Durham, NC. October 30, 1995.

Gillette, D.A. Research at Owens Lake, California. Presentation to the SORD, Air Resources Laboratory, Las Vegas, NV, December 4, 1995.

Gillette, D.A. Resuspension research at Owens (Dry) Lake, CA, NOAA Technical Seminar. Presentation at the Department of Energy, Las Vegas, NV, December 4, 1995.

Gillette, D.A. The real dirt about the atmosphere. Presentation at the local American Meteorological Society meeting, Research Triangle Park, NC, February 15, 1996.

Gillette, D.A. Measurements of summer 1995 to spring 1996 wind erosion at Jornada del Muerto. Presentation at the Friends of the Jornada Annual Meeting, Las Cruces, NM, May 23, 1996.

Gillette, D.A. Mechanique de la mise en mouvement des particules du sol sous l'action du vent: de l'erosion eolienne a la desertification (given in English). Association Universitaire de Mecanique, Creteil, France, September 4, 1996.

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Hunt, J.C.R. (Chief Executive, The Meteorological Office, England). Developments in forecasting the environment. Seminar presented at the Fluid Modeling Facility, Research Triangle Park, NC, January 30, 1996.

Irwin, J.S. Comparative evaluation of two air quality models: Within-regime evaluation statistic. Presentation at the 4th Workshop on Harmonisation with Atmospheric Dispersion Modelling for Regulatory purposes, , Oostende, Belgium, May 8, 1996.

LeDuc, S.K. Clouds. Presentation to the first-grade classes at Memorial Elementary School, Paris, IL, October 5, 1995.

LeDuc, S.K. Implications of global climate warming. Televised presentation on “30 Minutes,” WRAL-TV, taped February 9, 1996, aired February 11, 1996.

LeDuc, S.K. Remote sensing. Presentation to the seventh-grade classes at A.L. Stanback Middle School, Hillsborough, NC, March 11, 1996.

LeDuc, S.K. Emissions modeling and visualization tools — Current and future. Televised workshop, North Carolina State University, Raleigh, NC, April 23, 1996.

LeDuc, S.K. Comparing model predictions to satellite data. Presentation at the Second International Symposium on Spatial Accurancy in Natural Resources and Environmental Sciences, Ft. Collins, CO, May 22, 1996.

LeDuc, S.K. Remote sensing and clouds from computers. Presentation to the third-grade class at Swift Creek Elementary School, Raleigh, NC, May 29, 1996.

LeDuc, S.K. Computational atmospheric science: Preparing for Models-3. Televised workshop, North Carolina State University, Raleigh, NC, July 10, 1996.

Lee, R.F., and J.S. Touma. Air pollution meteorology. Presentation to the seventh-grade classes at Githens School, Durham, NC, April 2, 1996.

Novak, J.H. EPA’s HPCC FY-1998 Program. Presentation at the Computing, Information, and Communications Research and Development Subcommittee of the National Science and Technology Council, Washington, DC, September 4, 1996.

Novak, J.H. Trends and directions for HPCC at EPA. Presentation at the RCI North American Annual Membership Executive Conference, Reston, VA, October 31, 1995.

Novak, J.H. Quality assurance for development of EPA’s Models-3. Presentation to the National Technical Workshop on Quality Assurance in Information Technology, Research Triangle Park, NC, August 21, 1996.

Novak, J.H. EPA/HPCC program and opportunities for collaboration. Presentation to NASA representatives, Research Triangle Park, NC, March 1, 1996.

Ohba, M. (Tokyo Institute of Polytechnics, Japan) Field and wind-tunnel study of air-change rates in a house using video images. Seminar presented at the Fluid Modeling Facility, Research Triangle Park, NC, July 25, 1996.

Okabayashi, K. (Mitsubishi Heavy Industries, Japan) Estimation of maximum GLC's with long averaging times over terrain using wind-tunnel model studies. Seminar presented at the Fluid Modeling Facility, Research Triangle Park, NC, June 21, 1996.

Petersen, W.B., and G.H. Crescenti. Strategic Environmental Research and Develoment Program (SERDP). Briefing for the SERDP Panel at Alexandria, VA, May 15, 1996.

Pierce, T.E. Biogenic emission state-of-science and research needs. NARSTO Scientific Assessment Meeting, Dallas, April 17, 1996.

Pierce, T.E. Use of biogenic emissions in regulatory oxidant models. International Workshop for Biogenic Volatile Organic Compounds, Estes Park, CO, August 23, 1996.

Pierce, T.E. Meteorology. Presentation at the Green Elementary School, Raleigh, NC, August 15, 1996.

Pierce, T.E. Research and development of emission inventories for the Southern Oxidants Study Nashville, TN, 1995 Experiment. Presentation at the Air & Waste Management Association Annual Meeting, Nashville, TN, June 27, 1996.

Pierce, T.E. Biogenic emissions research in the United States. US/German/European Community Workshop on Ozone Modeling, Berlin, Germany, September 25, 1996.

Roselle, S.J. Archiving of SOS data. Presentation at the Southern Oxidants Study (SOS) Nashville Data Analysis Workshop, Raleigh, NC, May 9, 1996.

Roselle, S.J. The Models-3 aqueous chemistry module. Presentation at the Models-3 Science Workshop, Research Triangle Park, NC, September 19, 1996.

Roselle, S.J. Photolysis rate processor for Models-3. Presentation at the Models-3 Science Workshop, Research Triangle Park, NC, September 20, 1996.

Rottman, J.W. (Naval Research Laboratory, Washington, DC). Ship tracks in the sky. Seminar presented at the Fluid Modeling Facility, Research Triangle Park, NC, September 23, 1996.

Schere, K.L. Data management in NARSTO-NE. Presentation at the NARSTO-NE Assembly Meeting, Boston, MA, October 26, 1995.

Schere, K.L. NARSTO assessment process. Presentation at the 1995 Fall NARSTO Workshop, San Antonio, TX, November 14, 1996.

Schere, K.L. NARSTO update. Presentation at the 1995 AWMA-EPA Information Exchange, Research Triangle Park, NC, December 5, 1995.

Schere, K.L. EPA collaboration in the Southern Oxidants Study. Briefing for the Assistant Administrator for Research and Development, Office of Research and Development, U.S. Environmental Protection Agency, Washington, DC, March 15, 1996.

Schere, K.L. The interface of atmospheric sciences and air quality management: A U.S. perspective. Invited lecture at the 1996 EUROTRAC Symposium, Garmisch-Partenkirchen, Germany, March 27, 1996.

Schere, K.L. NARSTO assessment activities. Presentation at the SOS/Nashville Data Analysis Workshop, Raleigh, NC, May 6, 1996.

Schere, K.L. An overview of the North American research strategy for tropospheric ozone. Presentation at the 6th International Conference of the Israel Society for Ecology and Environmental Quality Sciences, Jerusalem, Israel, July 2, 1996.

Schere, K.L. The EPA/NARSTO program. Briefing for the Deputy Assistant Administrator for Science, Office of Research and Development, U.S. Environmental Protection Agency, Research Triangle Park, NC, July 17, 1996.

Schere, K.L. The NARSTO 1998 assessment. Presentation to the Ozone Transport Assessment Group, Washington, DC, July 23, 1996.

Schere, K.L. Air quality model development in the United States. Presentation at the Fifth U.S.-German Workshop on the Photochemical Ozone Problem and Its Control, Berlin, Germany, September 25, 1996.

Schere, K.L. The NARSTO 1998 assessment. Presented to the Air Quality Research Subcommittee of the CENR, Washington, DC, June 20, 1996.

Schiermeier, F.A. Opening address. Presentation at the Twenty-First NATO/CCMS International Technical Meeting on Air Pollution Modeling and Its Application, Baltimore, MD, November 6, 1995.

Schiermeier, F.A. Overview of NATO/CCMS International Technical Meetings on Air Pollution Modeling and Its Application. Presentation at State Department Meeting of NATO Alliance Countries, Washington, DC, November 13, 1995.

Schiermeier, F.A. In-house performance of scientific research. Presentation to the National Research Council Committee on Research and Peer Review in EPA, Research Triangle Park, NC, May 17, 1996.

Schiermeier, F.A. Description and availability of EPA air quality dispersion models. Presentation to the delegation of Thailand Government Environmental Officials hosted by the World Environment Center, Research Triangle Park, NC, August 20, 1996.

Shankar, U., and F.S. Binkowski. An integrated aerosol model to predict regional visibililty with output visualization. Presentation at the Fourteenth Annual Meeting of the American Association for Aerosol Research, Pittsburgh, October 10, 1995.

Snyder, W.H. Wind-tunnel measurements of two-dimensional entrainment in dense-gas flows through large roughness elements. PERF meeting, University of Surrey, Guildford, England, November 8, 1995.

Snyder, W.H. Wind-tunnel measurements of two-dimensional entrainment in dense-gas flows through large roughness elements. PERF meeting, University of Surrey, Guildford, England, January 10, 1996.

Snyder, W.H. Wind-tunnel measurements of two-dimensional entrainment in dense-gas flows through large roughness elements. PERF meeting, University of Surrey, Guildford, England, May 21, 1996.

Thompson, R.S. Laboratory simulation of the rise of buoyant thermals. Seminar presented at the Fluid Modeling Facility, Research Triangle Park, NC, June 4, 1996.

Walter, G. Jump starting the Internet at NOAA in RTP. NOAA Web Conference, Washington, DC, June 25, 1996.

Wilson, R., and S.G. Perry. Status report on AERMOD model development project. Presentation at the Regional and State Modelers Workshop, Research Triangle Park, NC, April 24, 1996.

Young, J. Optimizing gas-phase chemistry solver for massively parallel processing on the Cray T3D. Presentation at the Twenty-First NATO/CCMS International Technical Meeting on Air Pollution Modeling and Its Application, Baltimore, Maryland, November 6-8, 1995.

Zelenka, M.P. Hazardous Air Pollutant Exposure Model for mobile sources. Presentation at the Regional/State/Local Agency Modeler's Workshop, Research Triangle Park, NC, April 24, 1996.

Zelenka, M.P. A synoptic climatology of fine particle acid aerosols. Presentation at the Measurement of Toxic and Related Air Pollutants Symposium, Research Triangle Park, NC, May 8, 1996.

Zhu, GuWei (M.S. student, NCSU). A wind-tunnel investigation of the flow structure within a dense gas plume. Seminar presented at the Fluid Modeling Facility, Research Triangle Park, NC, May 1, 1996.

APPENDIX D: WORKSHOPS

International Conference on Atmospheric Ammonia. Culham, Oxford, England, October 2-4, 1995.

F.S. Binkowski

Chesapeake Bay Shared Resources Conference/Workshop, Warrenton, VA, October 10-12, 1995.

R.L. Dennis

HPCC Program Computer Systems Briefing, Washington, DC, October 11-12, 1995.

J.H. Novak

OFCM Meeting of Working Group on Climate Services, Silver Spring, MD, October 12-13, 1995.

S.K. LeDuc

Workshop on Soil NO_x Emissions, Raleigh, NC, October 16, 1995.

K.L. Schere

North American Research Strategy for Tropospheric Ozone Fall Planning Workshop, San Antonio, TX, November 13-17, 1995.

R.L. Dennis
T.E. Pierce
K.L. Schere

OTAG Implementation Strategies Issues Workgroup, Washington, DC, November 19, 1995.

N.C. Possiel

6th PERF 93-16 Workshop, EPA/Exxon, Research Triangle Park, NC, January 16-17, 1996.

W.B. Petersen
G.A. Briggs

Advisory Committee Meeting for the Great Lakes Agricultural Profile Project, Ann Arbor, MI, January 31, 1996.

W.G. Benjey

NARSTO-NE Executive Steering Committee Meeting, Washington, DC, March 5, 1996.

K.L. Schere

Chesapeake Bay Air Quality Coordination Group Workshop, Annapolis, MD, March 12-13, 1996.

R.L. Dennis

Regression Analysis Workshop, Research Triangle Park, NC, March 13, 1996.

B.K. Eder

Endocrine Disruptor Exposure Workshop, Compartmental Model Panel, Research Triangle Park, NC, March 14, 1996.

A.H. Huber
E.J. Cooter

1996 EUROTRAC Symposium, Garmisch-Partenkirchen, Germany, March 25-29, 1996.

K.L. Schere

Annual States/EPA Region 6 Air Quality Modeling Workshop — Telephone Briefing, Dallas, TX, March 27-28, 1996.

D.A. Atkinson
R.F. Lee
J.S. Touma

Development of Calibration and Data Validation Procedures, Reno, NV, March 28, 1996.

G.A. Briggs

Project MOHAVE Data Review Workshop, Las Vegas, NV, April 1-4, 1996.

J.K.S. Ching

NSTC/CENR Mid-Atlantic Region Pilot Workshop, College Park, MD, April 9-12, 1996.

R.L. Dennis
P.L. Finkelstein

Dispersion Modeling for Risk Management Programs, Carolinas Air Pollution Control Association, Ashville, NC, April 12, 1996.

J.S. Touma

North American Research Strategy for Tropospheric Ozone Analysis and Assessment Workshop, Dallas, TX, April 16-19, 1996.

R.L. Dennis
T.E. Pierce
K.L. Schere

South Florida Mercury Research Coordination Workshop, Orlando, FL, April 22-24, 1996.

O.R. Bullock, Jr.

Regional/State/Local Modelers Workshop, Research Triangle Park, NC, April 22-26, 1996.

D.A. Atkinson
D.T. Bailey
G.H. Crescenti
J.S. Irwin
B.L. Orndorff
S.G. Perry
W.B. Petersen
J.S. Touma
M.P. Zelenka

Fourth Supercomputer Workshop, National Institute for Environmental Studies, Tsukuba, Japan, April 23-26, 1996.

D.W. Byun

Annual Spring Meeting of Korean Meteorological Society, Chunchon, Korea, April 26-29, 1996.

D.W. Byun

NOAA Mesoscale Modeling Workshop, Research Triangle Park, NC, May 1-2, 1996.

W.G. Benjey
D.W. Byun
J.K.S. Ching
R.L. Dennis
J.H. Novak
S.K. LeDuc
J.A. Pleim
K.L. Schere

OTAG Regional and Urban Modeling Workgroup, Washington, DC, May 2-3, 1996.

N.C. Possiel

SOS-Nashville Data Analysis Workshop, Raleigh, NC, May 6-10, 1996.

T.E. Pierce
S.J. Roselle
K.L. Schere

NARSTO Science and Resource Planning Group Meeting, Gaithersburg, MD, May 22, 1996.

K.L. Schere

Interim Evaluation of PERF Dense Gas Diffusion Wind Tunnel Experiments, University of Surrey, England, May 21-22, 1996.

G.A. Briggs

Sixth International Global Emissions Inventory Activities Workshop, Toronto, Canada, May 25-31, 1996.

W.G. Benjey

EPA National Environmental Supercomputing Center Scientific Working Group Meeting, Bay City, MI, June 12-13, 1996.

J.H. Novak

OTAG Regional and Urban Modeling Workgroup, Washington, DC, June 12-13, 1996.

N.C. Possiel

6th International Conference of the Israel Society for Ecology and Environmental Quality Sciences, Jerusalem, Israel, June 29-July 5, 1996.

K.L. Schere

IIASA Task Force on Environmental Change — Third Workshop, Laxenburg (Vienna), Austria, July 1-4, 1996.

R.L. Dennis

NorthEast States for Coordinated Air Use Management (NESCAUM) Mercury Workshop, Kennebunkport, ME, July 8-9, 1996.

O.R. Bullock, Jr.

Symposium on Air Quality Measurements, Dedham, MA, July 10-11, 1996.

J.K.S. Ching

Sixth PSU/NCAR Mesoscale Model Users Workshop, Boulder, CO, July 22-24, 1996.

J.K.S. Ching
J.E. Pleim

EPA Dioxin Workshop on Deposition and Reservoir Sources, Washington, DC, July 22-24, 1996.

O.R. Bullock, Jr.

NARSTO Database Meeting, NASA Headquarters, Washington, DC, July 24, 1996.

K.L. Schere

OFCM Meeting of Working Group on Climate Services, Silver Spring, MD, July 24, 1996.

S.K. LeDuc

OTAG Regional and Urban Modeling Workgroup, Washington, DC, July 24, 1996.

N.C. Possiel

Gaseous Diffusion Plant Safety Analysis Report HGSYSTEM/UF6 Enhancements Review, Research Triangle Park, NC, August 7-8, 1996.

G.A. Briggs

Data Analysis Planning Meeting, Research Triangle Park, NC, August 9, 1996.

G.A. Briggs

National Science and Technical Council Meeting, Washington, DC, August 13, 1996.

J.H. Novak

National Technical Workshop on Quality Assurance and Information Management Chapel Hill, NC, August 20-22, 1996.

J.S. Irwin
B.K. Eder

International Workshop for Biogenic Volatile Organic Compounds, Estes Park, CO, August 22-23, 1996.

T.E. Pierce

Air Toxics Implementation Workshop, Research Triangle Park, NC, August 26-29, 1996.

J.S. Irwin
J.S. Touma

SOS Science Team Meeting, Raleigh, NC, September 12-13, 1996.

K.L. Schere

International Air Quality Advisory Board Meeting of the International Joint Commission, Washington, DC, September 17, 1996.

W.G. Benjey

Statistical Issues in Setting Air Quality Standards, Research Triangle Park, NC, September 18-19, 1996.

A.H. Huber
M.P. Zelenka

NERL Human Exposure Teams, Las Vegas, NV, September 18-19, 1996.

A.H. Huber

Statistical Workshop, Research Triangle Park, NC, September 18-19, 1996.

B.K. Eder

Models-3 Science Workshop, Research Triangle Park, NC, September 18-20, 1996.

F.S. Binkowski
D.W. Byun
J.K.S. Ching
B.K. Eder
J.M. Godowitch
J.E. Pleim
S.J. Roselle
K.L. Schere

Fifth U.S.-German Workshop on the Photochemical Ozone Problem and Its Control, Berlin, Germany, September 24-27, 1996.

T.E. Pierce
K.L. Schere

APPENDIX E: VISITING SCIENTISTS

1. Dr. Ingmar Ackermann
   Ford Research Center
   Aachen, Germany

Dr. Ackermann visited the Division from July 8 through 10, 1996, to discuss aerosol modeling and plan for future collaborative efforts.

2. Drs. Bernhard and Heike Vogel
   University of Karlsruhe
   Karlsruhe, Germany

Drs. Bernhard and Heike Vogel visited the Division on October 10, 1995, to discuss advanced air quality and meteorology model issues.

3. Messrs. Brian Bloomer and Ravi Srivastava
   Acid Rain Division
   U.S. Environmental Protection Agency
   Washington, DC

Messrs. Bloomer and Srivastava visited the Division during the period of August 1 through 28, 1996, to become familiar with Models-3 development and provide input regarding data from continuous emissions monitoring.

4. Dr. R.E. Britter
   Department of Engineering
   University of Cambridge
   Cambridge, England

Dr. Britter visited the Fluid Modeling Facility on August 14, 1996, for discussions on dense-gas modeling.

5. Italo Chiarabini
   Sarria Institute of Chemistry
   Universidad Ramon Llull
   Barcelona, Spain

Mr. Chiarabini visited the Division during the period of June 7 through August 24, 1996, and developed a prototype object-oriented Aqueous Chemistry Module.

6. Dr. Sergei Chicherin
   Main Geophysical Observatory
   7 Karbyshev Street
   St. Petersburg, Russia

Dr. Sergei visited the Division on March 7, 1996, to discuss work on improving Russian air dispersion models.

7. Dr. Fred Fehsenfeld
   NOAA Aeronomy Laboratory
   Boulder, CO

Dr. Jeremy Hales
Envair
Kennewick, WA

Drs. Fehsenfeld and Hales visited the Division on October 25, 1995, to participate in a meeting of the NARSTO International Technical Team Leaders. Final plans were made for a NARSTO International Meeting during November 1995 in San Antonio, TX.

8. Drs. Noor Gillani and Aristoo Biazar
University of Alabama-Huntsville
Huntsville, AL

Drs. Gillani and Biazar visited the Division from November 27 through 29, 1995, and from May 7 through 10, and from September 18 through 20, 1996, to collaborate on work being conducted for the Models-3 plume-in-grid project.

9. Dr. Heins Hass
Ford Research Center
Aachen, Germany

Dr. Hass visited the Division from July 8 through 10, 1996, to discuss European modeling programs in atmospheric chemistry.

10. Professor Julian C.R. Hunt, FRS
Chief Executive, Meteorological Office
Bracknell, Berkshire
England

Professor Hunt visited the Fluid Modeling Facility on January 30 and 31, 1996, for discussions of scientific issues.

11. Professor Sonia Kredenweis
Colorado State University
Fort Collins, CO

Professor Kredenweis visited the Division on July 1 and 2, 1996, to plan collaborative work on aerosol modeling.

12. Drs. Chong-Bum Lee and Yong-Gook Kim
Department of Environmental Science
Kangwon National University
Chuncheon, Korea

Drs. Lee and Kim visited the Division from July 24 through August 2, 1996. The objectives for the visit were to present a seminar on the application of UAM for the simulation of ozone in the Seoul Metropolitan Area, and to discuss issues related to urban and regional air quality modeling using UAM and RADM.

13. Dr. Guenther Mauersberger
Technical University of Brandenburg-Berlin
Air Chemistry Work Group
Cottbus, Germany

Dr. Mauersberger visited the Division from July 17 through 19, 1996, to discuss his work on the full coupling of gas-phase and aqeous-phase chemistry in air quality models. During his visit, he gave a seminar and discussed the chemical process research for Models-3 with several of the Models-3 development team members.

14. Dr. Richard T. McNider
University of Alabama-Huntsville
Huntsville, AL

Dr. McNider visited the Division on July 30 and August 1, 1996, for discussions on using satellite data in specifying cloud fields for computing photolysis rates and for specifying surface solar radiation.

15. Professor M. Ohba
Tokyo Institute of Polytechnics
Tokyo, Japan

Professor Ohba visited the Fluid Modeling Facility on April 1, 1996, and again on July 25 and 26, 1996, to discuss wind tunnel modeling.

16. Dr. K. Okabayashi
Mitsubishi Heavy Industries
Nagasaki, Japan

Dr. Okabayashi visited the Fluid Modeling Facility on June 21, 1996, for discussions on wind-tunnel modeling.

17. Messrs. W. Pendergrass, R. White, and M. Hall
Atmospheric Turbulence and Diffusion Division
National Oceanic and Atmospheric Administration
Oak Ridge, TN

Messrs. Pendergrass, White, and Hall visited the Fluid Modeling Facility on April 2, 1996, for discussions on wind-tunnel modeling.

18. Dr. George Hidy
CE-CERT
University of California-Riverside
Riverside, CA

Dr. Hidy visited the Division on March 14, 1996, to discuss the NARSTO assessment with several Division members.

19. Professor Sara Pryor and Dr. Beki Barthelmie
Indiana University
Bloomington, IN

Professor Pryor and Dr. Barthelmie visited the Division on April 8 and 9, 1996, to discuss aerosol modeling and presented a seminar on field measurements taken in the Lower Fraser Valley in British Columbia, Canada.

20. Mr. Bret Schichtel
Washington University
St. Louis, MO

Mr. Schichtel visited the Division on June 12 and 13, 1996, to review progress on a cooperative agreement entitled *Three-Dimensional Monte Carlo Module for Interactive Trajectory Analysis*.

21. Mr. Trevor Scholtz
    Ortech International
    Missasuagua, Ontario, Canada

Mr. Scholtz visited the Division on October 12, 1995, to present a seminar and discussion on his developments in regional and global modeling of pesticide emissions in conjunction with the Atmospheric Environment Service Canada. He is working with Division scientists on modeling of atrazine deposition in the Great Lakes area.

22. Professor Herman Sievering
    University of Colorado
    Denver, CO

Professor Sievering visited the Division on July 15, 1996, to discuss evaluation of RPM and Models-3 aerosol results.

23. Dr. Itsushi Uno
    National Insititute for Environmental Studies
    Tsukuba, Japan

Dr. Uno visited the Division from September 8 through 20, 1996, to continue collaborative studies on the regional- and urban-scale air quality modeling, especially for the Models-3 project.

24. Dr. J.C. Weil
    Cooperative Institute for Research
    in Environmental Sciences (CIRES)
    University of Colorado
    Boulder, CO

Dr. Weil visited the Fluid Modeling Facility on several occasions (March 13 and 14, June 4 and 5, July 11 and 12, and September 3 through 6, 1996) for intensive discussions on the Open Burning/Open Detonation project being conducted in the water channel and the plume penetration of elevated inversion investigations being carried out in the convection tank.

25. Dr. J.C. Weil
    Cooperative Institute for Research
    in Environmental Sciences (CIRES)
    University of Colorado
    Boulder, CO

    Dr. Akula Venkatram
    University of California-Riverside
    Riverside, CA

Drs. Weil and Venkatram visited the Division from September 24 through 26, 1996, to attend the meeting of the AERMIC workgroup.

26. Professors J. Wyngaard and J. Brasseur
Department of Mechanical Engineering
The Pennsylvania State University
University Park, PA

Dr. K. Wilson
Army Research Laboratory
White Sands, NM

Professors Wyngaard and Brasseur, and Dr. Wilson visited the Fluid Modeling Facility on April 29, 1996, for discussions and demonstrations of plume penetration of elevated inversions in the convection tank.

APPENDIX F: UNDERGRADUATE AND GRADUATE STUDENTS AND POSTDOCTORAL RESEARCHERS

1. Mr. Ryan Boyles
   North Carolina State University
   Raleigh, NC

   Mr. Clint Tillerson
   North Carolina State University
   Raleigh, NC

Messrs. Boyles and Tillerson, students at North Carolina State University, Raleigh, North Carolina, were interns during summer 1996. Mr. Boyles participated in the NOAA summer student program. Mr. Tillerson worked through an EPA/NCSU cooperative agreement subcontracted to Shodor Education Foundation, Durham, NC. During their twelve week assignment, Boyles and Tillerson developed an on-line meteorology course with focus on air quality modeling.

2. Donna A. Cunningham
   University of North Carolina at Chapel Hill
   Chapel Hill, NC

Miss Cunningham, a freshman at the University of North Carolina at Chapel Hill, was a participant in the Order of the Bell Tower Extern Program, which matches students with alumni during spring break for the oppportunity to explore careers and learn more about their fields of interests. Miss Cunningham spent part of the 1996 spring break working in the Division Library with an alumna and rotating through some of the library's functions.

3. Ms. Jianfeng (Deborah) Ding
   Department of Marine, Earth and Atmospheric Sciences
   North Carolina State University
   Raleigh, NC

Ms. Ding is a master of science candidate completing her second year at the Fluid Modeling Facility. She has completed wind tunnel measurements on the intermittency of turbulence within a dense-gas plume and its transition to a laminar state at small Reynolds numbers. A data report and thesis are in preparation.

4. Dr. Jie Lu
   The Pennsylvania State University
   University Park, PA

Dr. Lu, postdoctoral researcher, completed his second year at the Fluid Modeling Facility where he is studying plume penetration of elevated inversions in the convection tank. The work is being done in collaboration with Dr. J.C. Weil, CIRES, University of Colorado, Boulder, CO, and Dr. John Wyngaard, The Pennsylvania State University, University Park, PA. Dr. Lu was instrumental in developing subsystems for concentration measurements in the convection tank using laser induced fluorescence.

APPENDIX G: ATMOSPHERIC SCIENCES MODELING DIVISION STAFF FY-1996

All personnel are assigned to the U.S. Environmental Protection Agency from the National Oceanic and Atmospheric Administration, except those designated EPA, who are employees of the Environmental Protection Agency, or PHS, who are members of the Public Health Service Commissioned Corps.

Office of the Director

Francis A. Schiermeier, Supervisory Meteorologist, Director
Herbert J. Viebrock, Meteorologist, Assistant to the Director
Dr. Robin L. Dennis, Physical Scientist
Dr. Basil Dimitriades (EPA), Physical Scientist
Dr. Peter L. Finkelstein, Physical Scientist
Bruce W. Gay, Jr. (EPA), Program Manager
Evelyn M. Poole-Kober, Technical Editor
Barbara R. Hinton (EPA), Secretary
B. Ann Warnick, Secretary

Atmospheric Model Development Branch

Dr. Jason K.S. Ching, Supervisory Meteorologist, Chief**
Dr. Francis S. Binkowski, Meteorologist
O. Russell Bullock, Jr., Meteorologist**
Dr. Daewon W. Byun, Physical Scientist
Dr. John F. Clarke, Meteorologist
Dr. Brian K. Eder, Meteorologist
James M. Godowitch, Meteorologist
Dr. Jonathan E. Pleim, Physical Scientist
Shawn J. Roselle, Meteorologist
Kenneth L. Schere, Meteorologist
Tanya L. McDuffie, Secretary

Fluid Modeling Branch

Dr. William H. Snyder, Supervisory Physical Scientist, Chief
Dr. Dale A. Gillette, Physical Scientist
Robert E. Lawson, Jr., Physical Scientist
CDR. Roger S. Thompson (PHS), Environmental Engineer

Modeling Systems Analysis Branch

Joan H. Novak, Supervisory Computer Specialist, Chief
Dr. William G. Benjey, Physical Scientist
Dr. Sharon K. LeDuc, Physical Scientist
Thomas E. Pierce, Meteorologist
John H. Rudisill, III, Equipment Specialist
Alfreida R. Torian, Computer Specialist
Gary L. Walter, Computer Scientist
Dr. Jeffrey O. Young, Mathematician
Carol C. Paramore, Secretary (Since May 1996)

Applied Modeling Research Branch

William B. Petersen, Supervisory Physical Scientist, Chief
Dr. Gary A. Briggs, Meteorologist
Dr. Ellen J. Cooter, Meteorologist
Gennaro A. Crescenti, Physical Scientist
Dr. Alan H. Huber, Physical Scientist
Dr. Steven G. Perry, Meteorologist**
Donna B. Schwede, Physical Scientist
John J. Streicher, Physical Scientist
Lawrence E. Truppi, Meteorologist
Dr. Michael P. Zelenka, Meteorologist
Sherry A. Brown, Secretary

Air Policy Support Branch

John S. Irwin, Supervisory Meteorologist, Chief**
Dennis A. Atkinson, Meteorologist*
Dr. Desmond T. Bailey, Meteorologist
Russell F. Lee, Meteorologist
Brian L. Orndorff, Meteorologist
Norman C. Possiel, Jr., Meteorologist
Jawad S. Touma, Meteorologist

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*U.S. Environmental Protection Agency Community Environmental Protection Award
**U.S. Environmental Protection Agency Bronze Medal